



Indian Institute of Technology Bombay

Linear Alkyl Benzene

Group 15

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Executive Summary

This report presents the manufacturing process of Linear Alkylbenzene(LAB). Chapter 1 describes the chemical, its physical and chemical properties, uses of LAB and by-products formed during its manufacturing. Chapter 2 deals with various mechanisms, production processes, and proposed routes that are involved. After a short description, the yield of different routes is described.

Chapter 3 describes the challenges faced when using an old method and the ongoing research on it. Here, an overview of the global lab market of LAB is shown in terms of revenue. It provides an analysis of LAB-based products and their proportion in the market. It analyzes the size of this market for 14 years and the largest companies manufacturing it. At the end of this chapter, we have described that we are choosing Vadodara, Gujarat as the location for building the LAB production plant and the reasons behind it. Also, we have described the ideal plant capacity.

In Chapter 4, we have described the manufacturing process of LAB, taking Kerosene as our raw feed, inlet. This process can be split into two subprocesses, first the Front end process, which is the conversion of Kerosene into straight paraffin of the required carbons, i.e., 10 to 14. Then, the Back end process, deals with the conversion of that straight paraffin into LAB. The whole process is described with process flow diagrams.

In Chapter 5, we have done mass balance on reactors and separation columns. Mass of different components is shown in tabular form. Mass balance of the back end is shown.

In Chapter 6, simulation results of the complete backend process has been described. This is followed by comparison between results obtained from manual calculation and the simulation report.

In Chapter 7, we have described the results after doing sensitivity analysis for each equipment. This helps us in the choosing the right parameter to operate the equipments.

Acknowledgment

We would like to thank and express our gratitude to panel professors - Prof Hemant J Nanavati and Prof Pramod P Wangikar, Dept. of Chemical Engineering IIT Bombay - for their constant guidance and feedback throughout this project. Their continuous support has been immensely helpful for the successful completion of this project. They always drove us to the right path, in our research and presentations.

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Chapter 1

Linear Alkylbenzene

Linear Alkylbenzene(LAB), as shown in Figure 1.1, is a family of organic compounds with the formula of $C_6H_5-C_nH_{2n+1}$. Typically, $(n + m)$ lies between 10 and 14, although generally supplied as a tighter cut, such as C₁₂-C₁₅, C₁₂-C₁₃, and C₁₀-C₁₃, for detergent use. The alkyl group attached is unbranched. They are mainly produced as intermediate in the production of surfactants, for use in detergent. Its CAS No. is 67774-74-7 (Benzene, C₁₀-C₁₃ alkyl derivatives (LAB)) and has HS code 38170011.

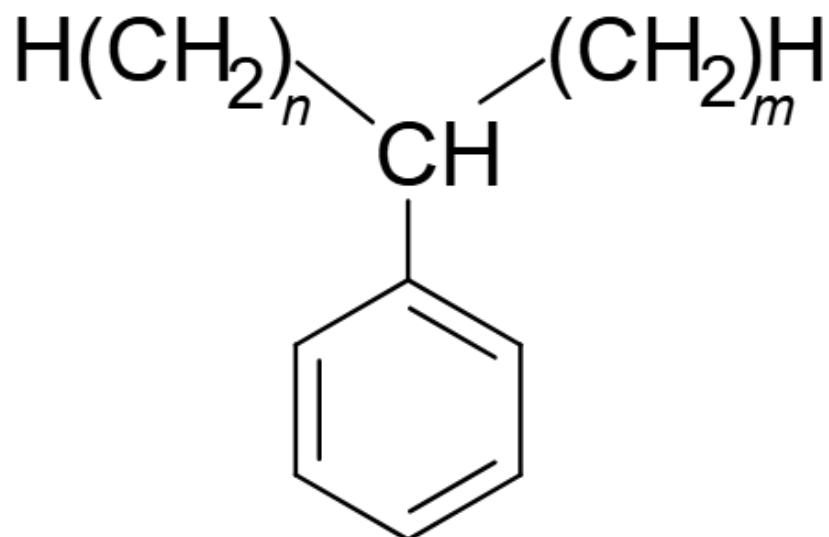


Figure 1.1: Linear Alkyl Benzene Molecule

1.1 Properties

Table 1.1 shows some of the physical and chemical properties of Linear Alkyl Benzene.

Table 1.1: Physical and Chemical Properties of LAB

Property Name	Property Value
Appearance	Clear colorless liquid
Odour	Odourless
Molecular Weight	239-245
Boiling Point (°C)	278-314
Melting Point (°C)	<-70
Solubility in Water	Insoluble
Solubility in Organic Solvent	Soluble (alcohol, ether)
Viscosity (cst @ 37.7 °C)	4.4
Density	0.86 g/cm ³
Bromine Index (mg Br ₂ /100g)	Max 10
Reactivity	Stable under normal conditions, but reacts with strong oxidizing agents

1.2 Uses of linear Alkylbenzene

Linear Alkylbenzene is mainly used as an intermediate in the production of surfactants and detergents. It is used in manufacturing many industrial and household cleansing materials:

1. It is sulphonated to produce linear alkylbenzene sulfonate(LAS), a biodegradable and widely used surfactant in detergents.
2. It is used in the dying process to improve the uniformity of color distribution.
3. It is used as an emulsifier in pesticide formulations, enhancing the effectiveness of agricultural chemicals.
4. It is used as a liquid scintillator in neutrino detection like in reactor Neutrino experiments.

1.3 Uses of By-products

1. It includes heavy alkylates, 95% molar hydrogen and aromatics.
2. Heavy alkylates(HAB) are used in secondary surfactant production.
3. Hydrogen is commercially used as fuel.

Chapter 2

Mechanism and Production Process

In the production of Linear Alkylbenzene (LAB), a Friedel-Craft alkylation reaction is used, where Lewis acids like aluminum chloride (AlCl_3) or hydrogen fluoride (HF) acts as the catalyst to attach a linear alkyl chain to a benzene molecule, essentially utilizing the electrophilic aromatic substitution mechanism to create the desired product, with HF being the more commonly used catalyst in modern industrial processes due to its superior selectivity and efficiency.

2.1 Routes for Linear Alkylbenzene production from paraffin

2.1.1 Route 1: Friedel Craft Alkylation using AlCl_3

As shown in Figure 2.1, the reaction starts with the conversion of paraffin into monochloroparaffin or alkyl chloride. This alkyl chloride reacts with AlCl_3 as Lewis acid, which forms carbocation by the removal of Cl^- as AlCl_4^- . The electrophile formed after this removal of Cl^- then acts as an electrophile, it attacks the benzene ring to form a sigma complex (called arenium ion). Finally, deprotonation restores aromaticity and yields linear alkylbenzene as the final product.[2]

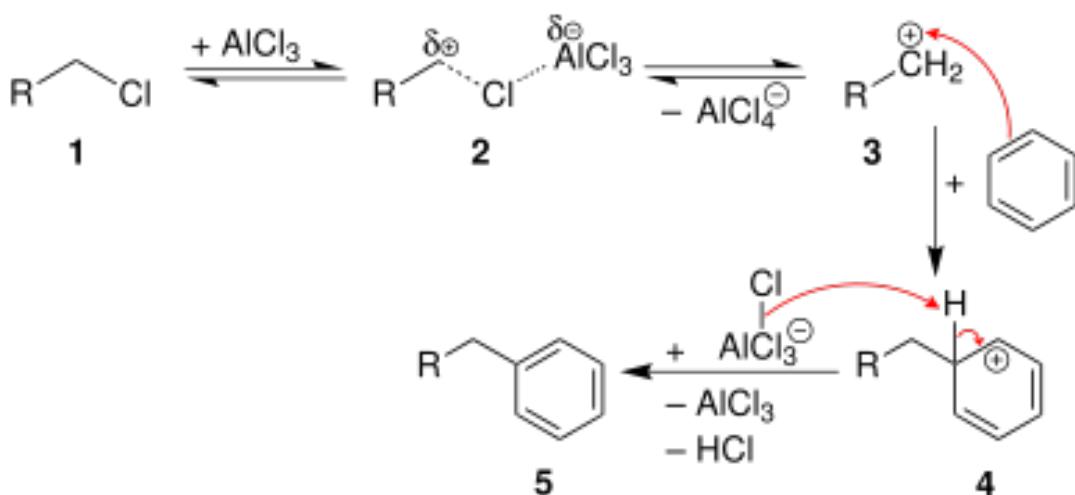


Figure 2.1: Friedel Craft Alkylation using AlCl_3 (used with permission)

2.1.2 Route 2: Friedel Craft Alkylation using HF

As shown in Figure 2.2, HF acts as both a catalyst and a promoter of carbocation formation. The linear alpha-olefin undergoes protonation by HF, it generates a highly reactive carbocationic intermediate at the benzylic or allylic position. This carbocation then attacks the benzene ring, which leads to the formation of a sigma complex (arenium ion). After rearrangement and deprotonation, a stable linear alkylbenzene (LAB) is formed, and HF is regenerated for continuous catalytic activity.[2]

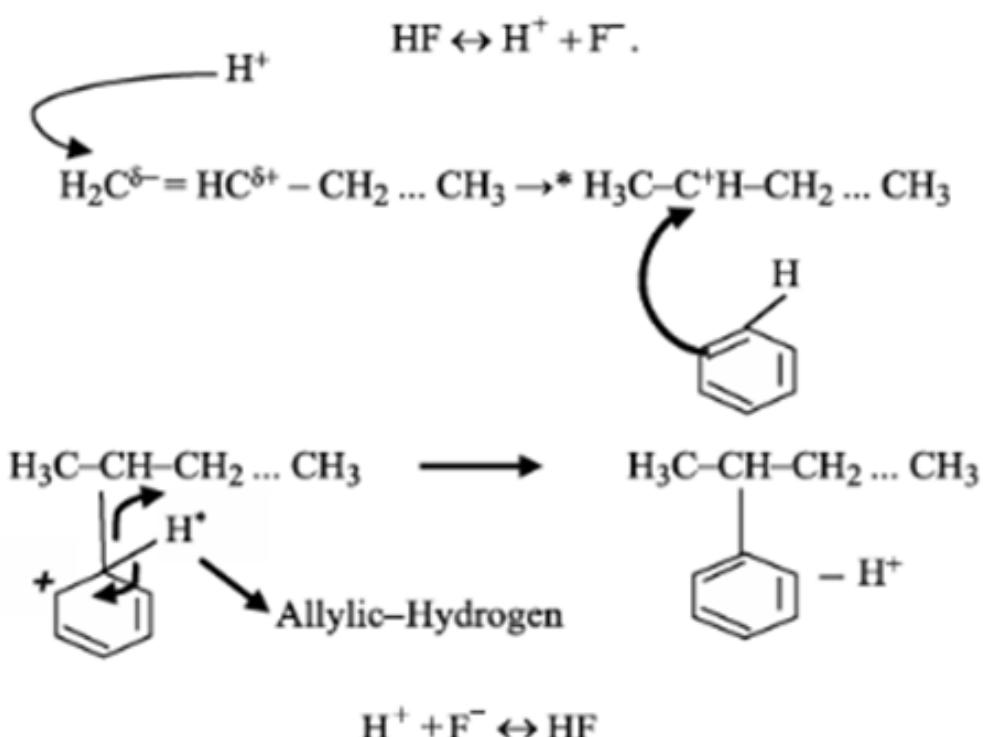


Figure 2.2: Friedel Craft Alkylation using HF(used with permission)

2.2 Various Production Processes

- Monochloroparaffin is formed by chlorination of Linear paraffins. AlCl_3 is used as catalyst which causes alkylation of benzene with monochloroparaffin. This method was used in early 1960s.
- Oligomerization of ethylene forms cracking waxes. Alkylation of these olefins with benzene results in production of LAB. It is done in presence of HCl catalyst.
- Olefins are formed after dehydrogenation of linear paraffins. It then reacts with benzene in the presence of HF acid catalyst.
- Detal process uses a solid catalyst. It includes degeneration of linear paraffin to olefins and reaction with benzene using fixed bed catalytic reactor.[1]

Chapter 3

Comparing Processes and Market Survey

3.1 Detal vs HF Process

1. Quality of products from HF and Detal are similar, but LAB produced from Detal is more linear and also leads to lower production of heavy alkylates.
2. Higher content of 2-phenylalkane is formed in Detal process which makes Linear alkylbenzene to be better sulphonated and to be used as surfactant.
3. For a LAB unit of 80,000 tons per year, cost estimates for Detal and HF systems were \$67 million and \$72 million, respectively, which makes Detal process more economical.[1]

3.2 Global production of LAB

Table 3.1 shows the different methods of production of LAB and their percentage globally.

Table 3.1: Production of LAB by Different Methods

Method	Production Percentage (%)
Chlorination and Alkylation	10
Dehydrogenation and Alkylation	81
Olefin with High Olefin Alkylation	9

- The dehydrogenation and HF alkylation method became quite popular because of its economic benefits and high-quality products.
- Normal paraffin dehydrogenation methods are generally preferred over other methods, due to the low cost of starting kerosene feed.
- However, in both processes of catalyzing using HF and AlCl_3 , the overall price of the company increases due to the transport of corrosive catalysts as well as downstream processing of acidic waste.

- Thus, it is beneficial to use heterogenous catalysts and there are ongoing research to enhance the performance of catalyst based alkylation[1]

3.3 Current Problems and Ongoing Research

1. Many acidic solids are active for the alkylation of benzene with different olefins. Though many catalysts are active, they commonly lack the required selectivity or stability.
2. Ionic liquids are a mixture of low melting point salts and they can be used to minimise corrosion in liquid alkylation system. The active catalyst is produced by adding AlCl₃ or other Lewis acids.
3. The ability to regenerate ionic liquid after a long time in the flow and the instability of these systems in water poses a challenge for using this technology.

3.4 Global LAB Market Overview

1. Asian market is experiencing growth, primarily because of increasing demand from the textile and leather industry for emulsification and dispersal purposes, as shown in Figure 3.1.
2. Growth is driven by increasing consumer spending on cleanliness and LAB's cost-effective, biodegradable properties as an intermediate for detergents and surfactants, as shown in Figure 3.2
3. The Linear Alkyl Benzene (LAB) market was valued at USD 10.9 billion in 2023 and is projected to grow at a CAGR of 4.30%, reaching USD 14.27 billion by 2032, as shown in Figure 3.3.

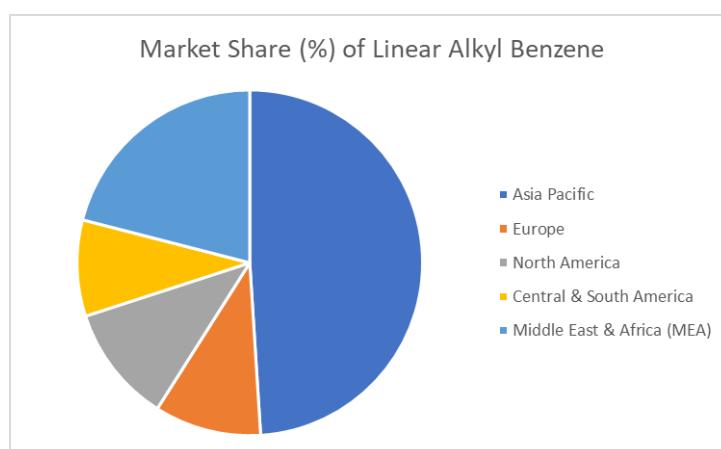


Figure 3.1: Global LAB market

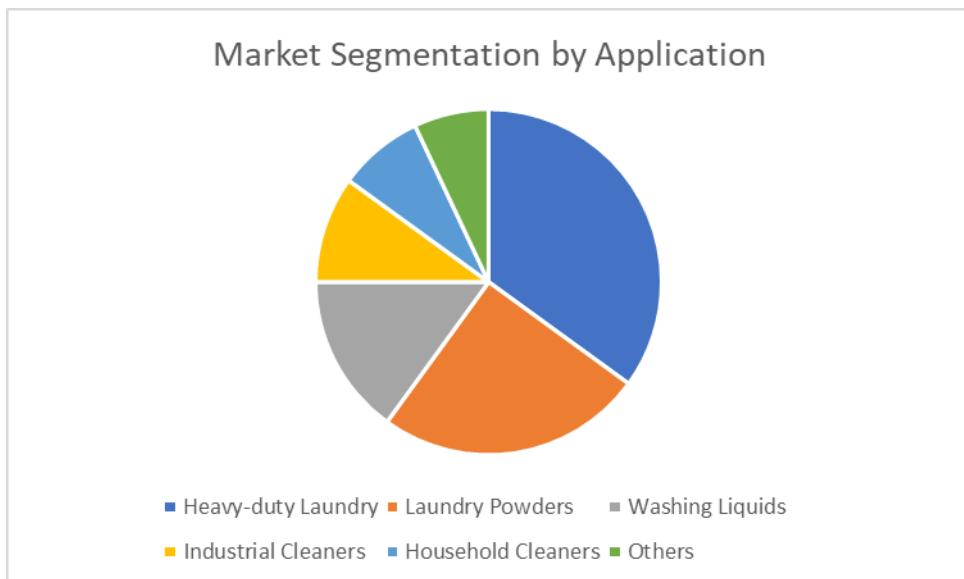


Figure 3.2: Global market segmentation

3.5 Market size and Major Producers

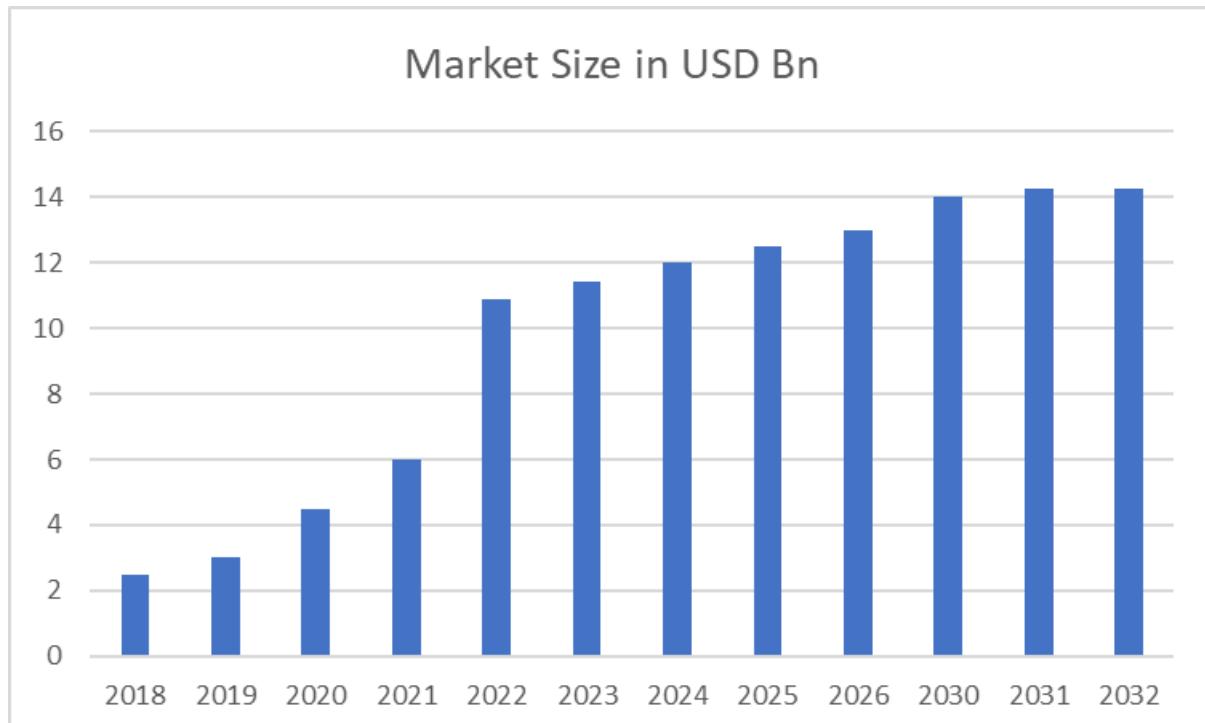


Figure 3.3: Market survey from 2018-2032



Figure 3.4: Major Producers

3.6 Desired location and Plant capacity

VADODARA, GUJARAT

1. Proximity to Refineries: The presence of IOCL's Gujarat Refinery in Vadodara offers feedstock supply and access to excellent industrial infrastructure.
2. As part of the Gujarat Industrial Development Corporation (GIDC) network, Vadodara benefits from a good industrial environment that supports chemical manufacturing.
3. The city offers a skilled labor pool in chemical and petrochemical sectors.

3.7 Plant capacity

An ideal capacity for a new LAB plant in India would be around 135,000 TPA. This recommendation is based on these factors:

- Indian LAB market achieved a total market volume of 536.78 thousand MT in 2024 and is expected to reach 655.83 thousand MT in 2030, with a projected Compound Annual Growth Rate (CAGR) of 3.43% through 2030.
- India's demand for LAB is rising because of the expanding detergent and cleaning products industry. India has experienced a supply-demand gap, leading to imports averaging around 225,000 tonnes over the past five years.

Existing Industry Benchmarks:

Tamilnadu Petroproducts Limited (TPL): TPL's plant in Manali, has a current capacity of 120,000 TPA, with plans to expand to 145,000 TPA by September 2024. This serves as basis for optimal plant capacity in the Indian context.

Chapter 4

Process Flow Diagram

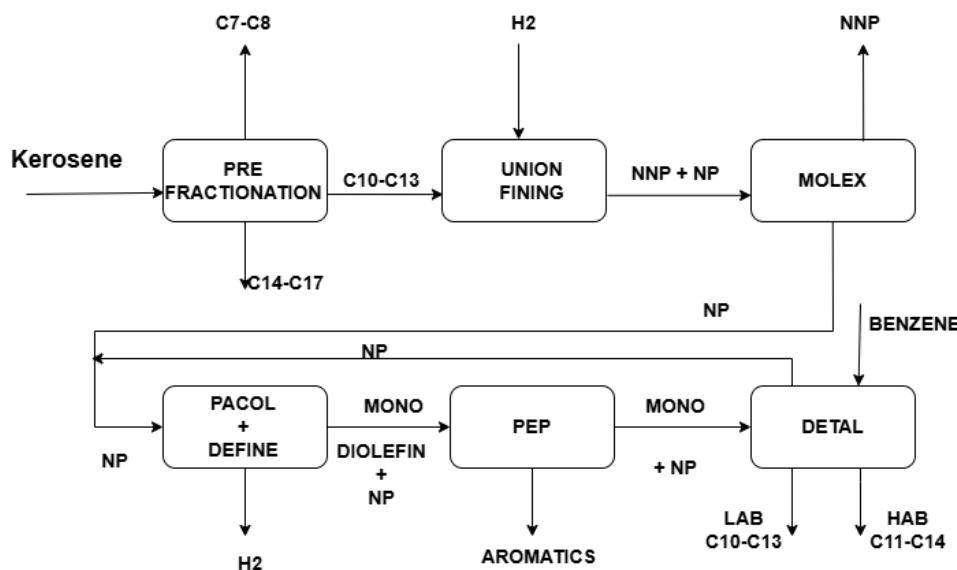


Figure 4.1: Block Diagram-Front end and back end

Front End

Production of Linear Alkylbenzene requires a special type of feed. To meet this specification, the input feed, which is Kerosene, must be processed to remove undesired hydrocarbon (both less light and heavier), impurities, and convert branched paraffins into branched paraffins.

This process is subdivided into three subprocesses as stated above:

1. Prefractionation
2. Union fining
3. MOLEX

Pre-fractionation - The feed here is straight-run Kerosene, which contains carbon range C7 to C17. The purpose is to separate hydrocarbons containing C10 to C14 from others. To achieve this one stripper column and one rerun column are required. The stripper column removes components up to C9 and Rerun column removes components from C15 to C17.

Union fining - Input from the previous process contains contaminants like Sulphur, Nitrogen, and, Metals compounds. It is here that these impurities are removed. Union fining is a catalytic, fixed bed process developed by UOP for hydro-treating a wide range of feedstocks. This process uses a catalytic hydrogenation method to upgrade the quality of petroleum fractions by removing sulfur, nitrogen, saturates olefin, and aromatic compounds. The Hydrotreater catalyst uses oxides of nickel and molybdenum on alumina bases as catalysts.

MOLEX - It is a very effective method to continuously separate normal paraffin from a stream of co-boiling hydrocarbons using physically selective adsorption. It simulates countercurrent contact between a fixed bed adsorbent and the feed stream.

This process contains three steps:

- Feed Adsorption
- Purification
- Desorption

4.1 PFD part-1(PACOL-Paraffin conversion to olefin)

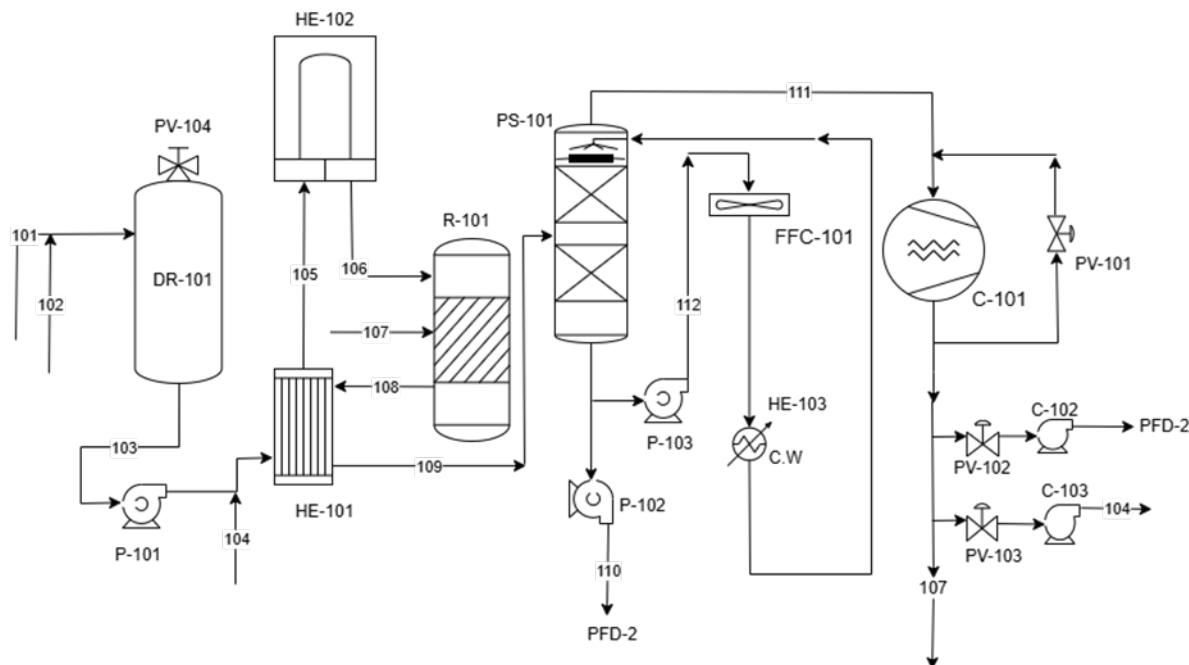


Figure 4.2: PFD part-1

Table 4.1: Stream Data Part-1

Stream No.	Composition	Conditions
101	N-Paraffin (fresh)	25-35°C
102	N-Paraffin (recycle)	170-180°C
103	N-Paraffin (fresh + recycle)	160°C
104	Recycle Hydrogen	45-55°C, 2.17 bar
105	N-Paraffin + Recycle Hydrogen	400°C
106	N-Paraffin + Recycle Hydrogen	450°C
107	Recycle Hydrogen	475°C
108	N-Paraffin + Hydrogen + Monolefins + Diolefins + Aromatics + Light Hydrocarbons (<C10)	210°C
109	N-Paraffin + Hydrogen + Monolefins + Diolefins + Aromatics + Light Hydrocarbons (<C10)	
110	N-Paraffin + Monolefins + Diolefins + Aromatics + Light Hydrocarbons (<C10)	
111	Hydrogen	

Following reactions occur in Pacol Reactor:

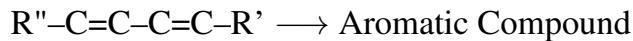
Olefin Formation



Diolefin Formation



Aromatics Formation



PFD description:

As per figure 4.1 and table 4.1, N-paraffin is fed to the Feed Surge Drum from tank farm(fresh) and recycled from detail Column. It is stored at 1.72 bar pressure and 160°C in the surge drum DR-101. Fresh paraffin is fed at a temperature of 30°C(stream 101), Recycled paraffin at 175°C(stream 102). The mixed paraffin is pumped to shell and tube heat exchanger HE-101 by pump P-101 at 150°C. This stream mixes with recycled hydrogen(stream 104) coming from screw compressor C-101 at 50°C and 2.16 bar. Its flow rate is controlled by spill back valve PV-101. The Feed and recycle gas stream enters the HE-101 and is heated up to 400°C and sent to Charge heater HE-102. The charge heater operates at 1000°C. It heats the stream up to 450°C. The stream enters the Pacol reactor R-101 which is a radial flow reactor and the catalyst used is stabilized platinum on alumina base in the form of cylindrical bed. Recycled hydrogen is injected into the reactor(stream 107). The reaction is endothermic and occurs at low pressure(1.37 bar). The Reactor product is sent to HE-101 and is cooled down to 210°C. This product is to be separated from hydrogen so it is sent to Product separator PS-101. The product stream enters the bottom portion of the vessel and passes through a packed bed. The vapor is cooled while passing up through the bed by cold recirculated liquid flowing down. As the vapor cools the condensable hydrocarbon (N-paraffin) it condenses and is collected at the bottom of the separator with the recirculated liquid (pumparound). The cold gas (hydrogen) then passes out through the top of the separator where it is returned to the C-101. The liquid collected at the bottom of the product separator is recycled by using Pump P-103 to the top of the product separator as pumparound liquid. The pump around liquid passes through fin fan cooler FFC-101 & then condenser HE-103. The flow of pumparound is controlled. The liquid containing unreacted paraffins, mono olefins, and diolefins is pumped to PFD-2 (Define reactor) by variable pump P-102. The hydrogen is allowed to evaporate and goes through the top of the vessel through stream 111 to the Recycle gas compressor C-101. The spill back valve PV-101 is used to control flow rate and pressure of the recycle hydrogen downstream.

The Recycle gas(hydrogen) is split into three streams: sent to PFD-2, into steam 104 and into R-101 pressurized by compressors C-102, C-103.

4.2 PFD part-2 (DEFINE- Di-olefin to olefin)

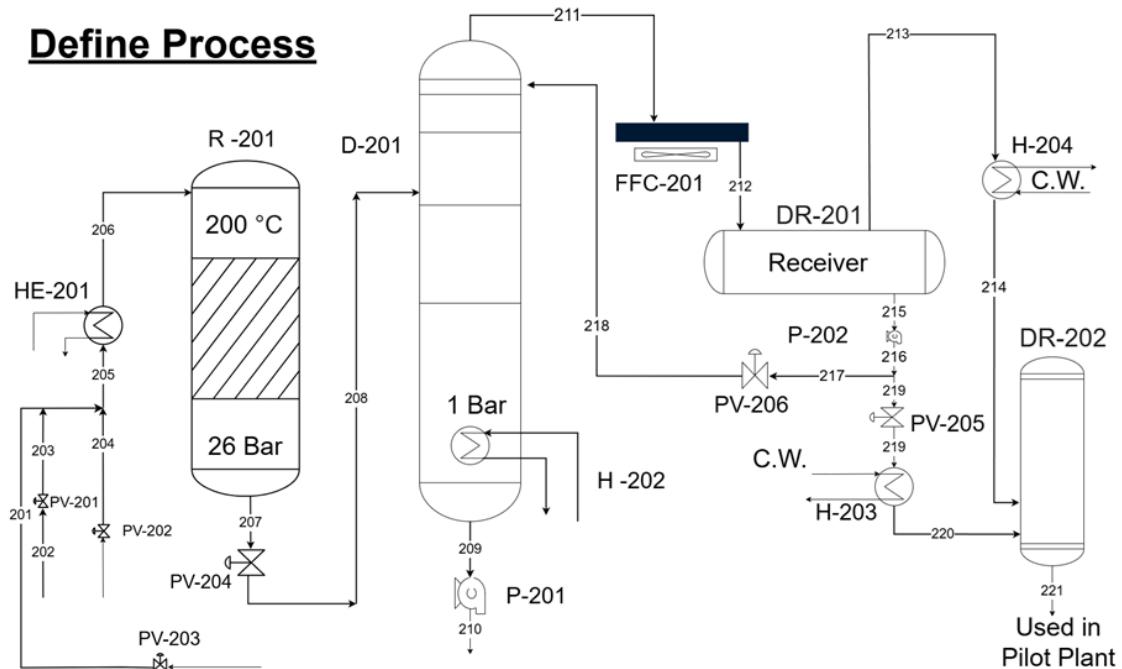


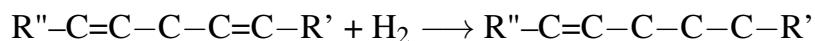
Figure 4.3: PFD part-2

Table 4.2: Stream Data Part-2

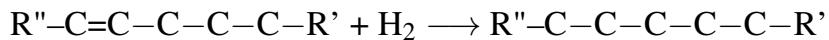
Stream No.	Composition	Condition
201	N-Paraffin, Olefin, Di-Olefin, Aromatic, Lower Hydrocarbon	34 Bar
202, 203	Sulfur	
204	Hydrogen	34 Bar
205	Hydrogen, Sulfur, N-Paraffin, Olefin, Di-Olefin, Aromatic, Lower Hydrocarbon	34 Bar
206	N-Paraffin, Olefin, Di-Olefin, Aromatic, Lower Hydrocarbon, Sulfur, Hydrogen	190-200°C
207-208	N-Paraffin, Olefin, Di-Olefin, Aromatic, Lower Hydrocarbon	190-200°C
209-210	N-Paraffin, Olefin, Di-Olefin, Aromatic, Lower Hydrocarbon (1%)	
211	Lower Hydrocarbon (99%)	
212	Lower Hydrocarbon (99%)	55°C
213-221	Lower Hydrocarbon	

Reactions:

1. Di-Olefin Hydrogenation (Main Reaction):



2. Mono-Olefin Hydrogenation (Side Reaction – Undesired):



Reaction Type:

- Exothermic (produces heat)

PFD description:

Feed from PFD 1 stream 110 (see figure 4.1 and table 4.2) containing paraffin, olefine, Di-olefin, aromatic and lower hydrocarbon is sent to define reactor through

stream 201, also from 202 sulfur is injected into the reactor and from stream 204 hydrogen is sent to the reactor (see figure 4.2).

After preheating the reactant using HE-201 at 190-200°C, it is sent to define reactor R-201.

Reaction occurs at 200°C and 26 bar pressure and this reaction converts di-olefin to olefin and a side reaction di-olefin converting to paraffin also takes place. This reaction has 90% conversion and 50% selectivity to olefin and 50% to paraffin.

After this product is sent to the D-201 distillation column, this distillation column separates lower hydrocarbon (99% from top) from the mixture.

After the separation olefin, paraffin, and di-olefin (remaining) is sent to the PEP column through stream 209 (see figure 4.2).

At the overhead of distillation column lower hydrocarbon is separated and sent to fin fan cooler to cool down stream at 55°C. Afterwards this is sent to the receiver drum DR-201 and then some amount is sent back to the distillation column to maintain the reflux ratio and other part containing remaining vapour and liquid is sent to fuel drum DR-202 wherein it is stored.

4.3 PFD part-3 (PEP-Pacol Enhancement Process)

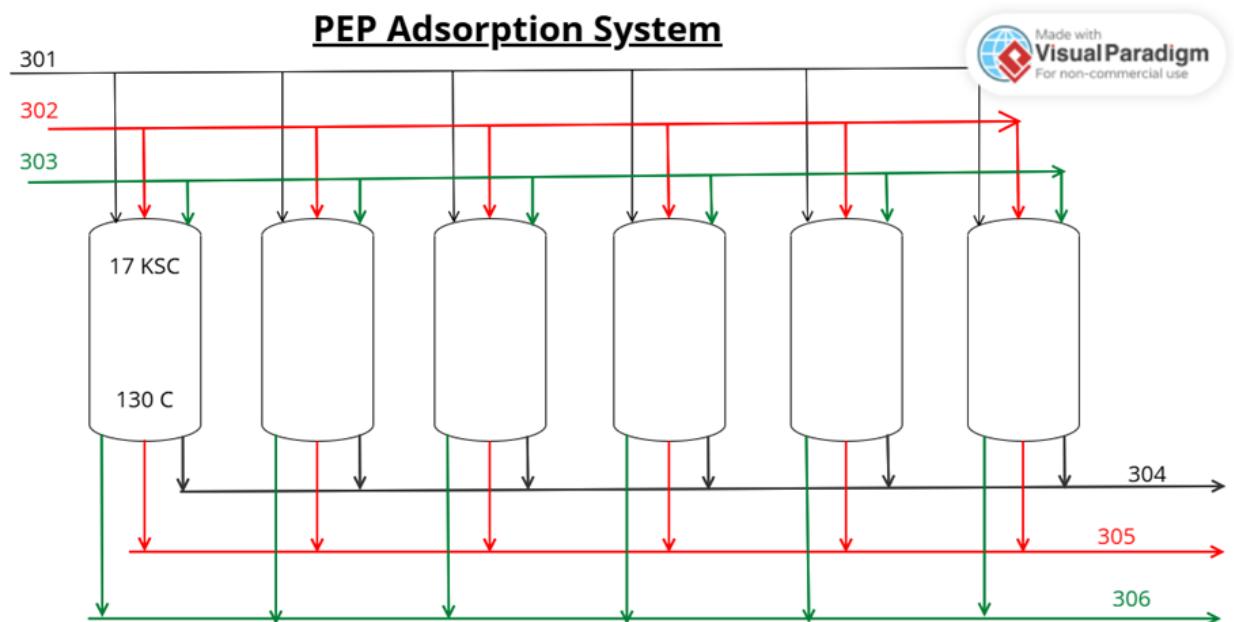


Figure 4.4: PFD part-3

Desorbant Column

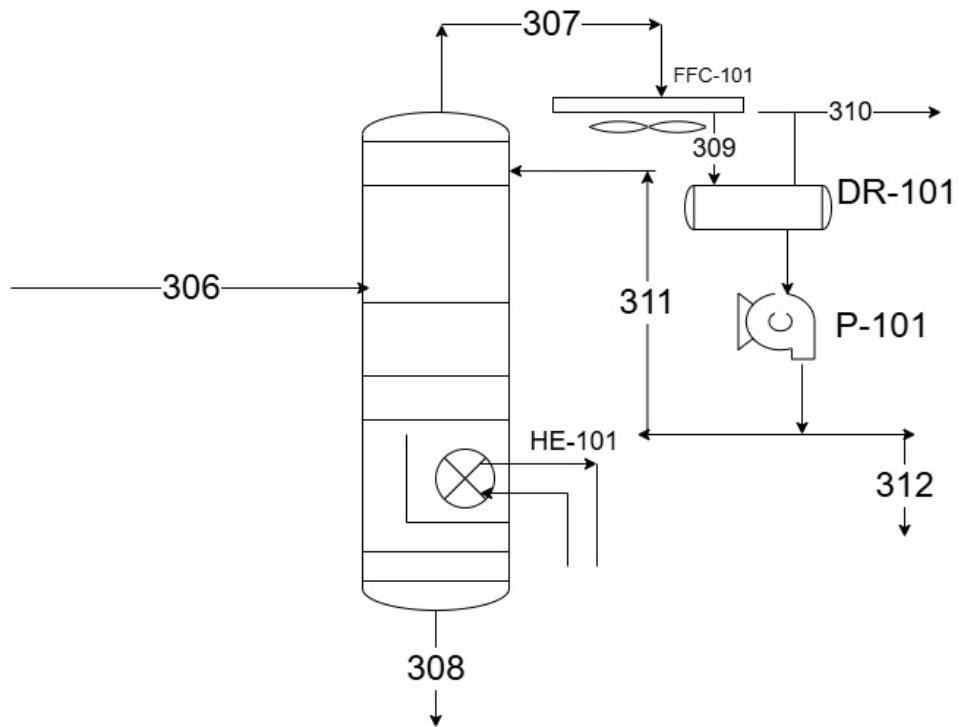


Figure 4.5: Desorbant Column

Depentanizer Column

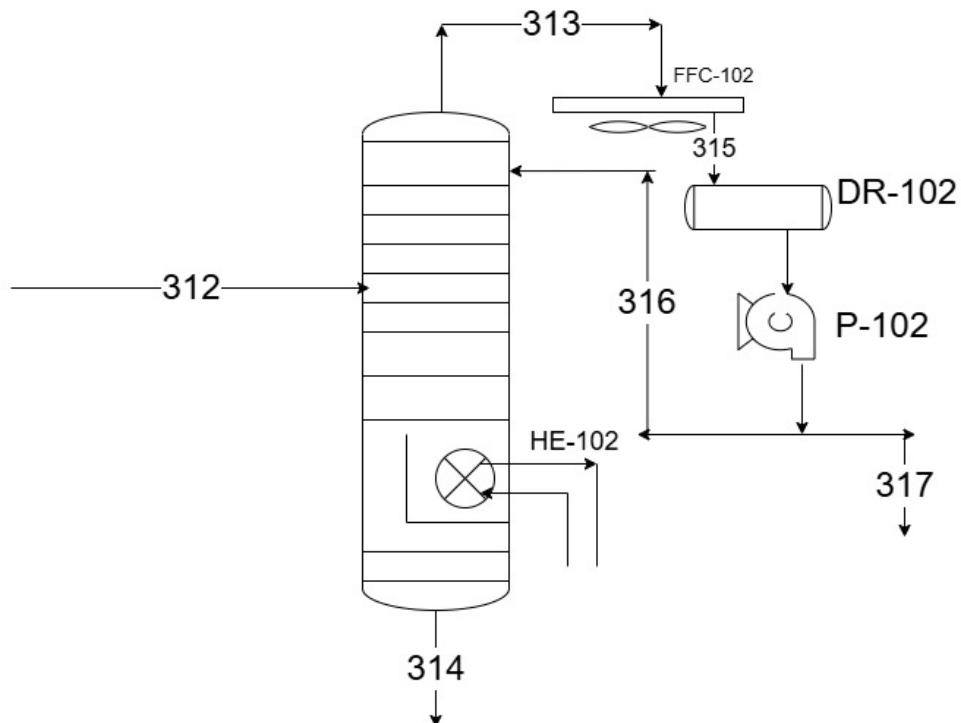


Figure 4.6: Depentanizer Column

Table 4.3: Stream Data Part-3

Stream No.	Composition
301	Paraffin,olefin and Aromatic Compounds
302,315,316	n-Pentane
303	Benzene
304	Paraffin and olefin
306	Benzene,Pentane,Aromatic Compounds
307,309,311,310,312	Benzene and n-Pentane
308	Aromatic Compounds
313, 317	Benzene and n-Pentane
314	Benzene, Paraffin,olefin

The main aim of this step is to remove the unwanted aromatics from the feed.

As shown in figure 4.3 and table 4.3, the untreated feed comes from stream (301) which is stream 210. It comes as the bottom outlet from the Define Process containing paraffins, olefins and aromatics. To separate aromatics from this feed, it is passed through adsorbers (zeolites pellet shaped) which act as molecular sieve on which aromatics get adsorbed. Initially, the adsorber vessels contain benzene and stream (301) displaces benzene to the desorbant column. When the feed is passed through the adsorbers, the aromatics get attached to the adsorbers. The treated feed containing paraffins and olefins is sent to the reactor(DETAL process) through stream (304) and is not passed to any of Desorbent and Depentanizer column.

To prevent loss of useful feed, n-pentane is introduced as purge through stream (302) to push treated feed out. n-Pentane removes the remaining treated feed but does not desorb aromatics. Now benzene is sent to the adsorbers in excess through stream (303) to desorb aromatics and the already present n-pentane (and some treated feed) in the adsorber gets displaced by benzene to depentanizer column (figure 4.6) through stream (305) as inlet stream 312 for separation of n-pentane and treated feed (contains traces of benzene as well). Treated feed is sent to Detal reactor while the n-pentane is recycled back to the system.

After n-pentane is completely displaced by benzene, untreated feed comes in and displaces the benzene stream containing aromatics and traces of n-pentane to desorbant column (figure 4.5) through stream (306). In desorbant column, the distillation column separates aromatics (from bottom) and benzene and n-pentane (from top). This benzene and n-pentane mixture is then sent to depentanizer column for separation of n-pentane and benzene. n-Pentane is recycled back to system while benzene is sent to Detal reactor.

As we can see from the above description there is a continuous cycle of events of adsorption and desorption of aromatics that removes the unnecessary aromatics from the reactant feed.

4.4 PFD Part-4:(DETAL:Detergent Alkylation Unit)

4.4.1 Detal Reactor

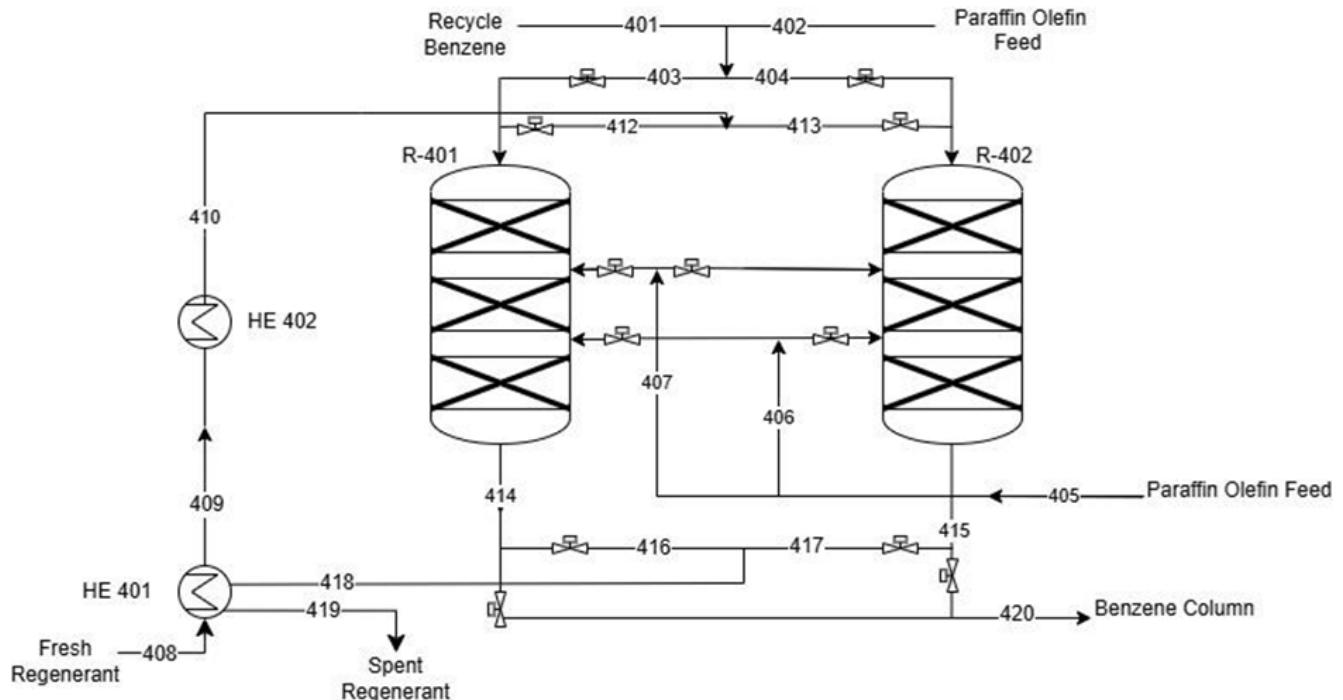


Figure 4.7: PFD part-4

Table 4.4: Stream Data Part-4

Stream No.	Composition
401	Benzene
402, 405, 406, 407	Paraffin Olefin Feed
403, 404	Benzene and Paraffin Olefin Feed
408, 409, 410, 413	Fresh Regenerator (Benzene)
414, 420	LAB, Paraffin, Heavy Alkylates
415, 417, 418, 419	Spent Regenerator (Benzene)

4.4.2 Benzene Column

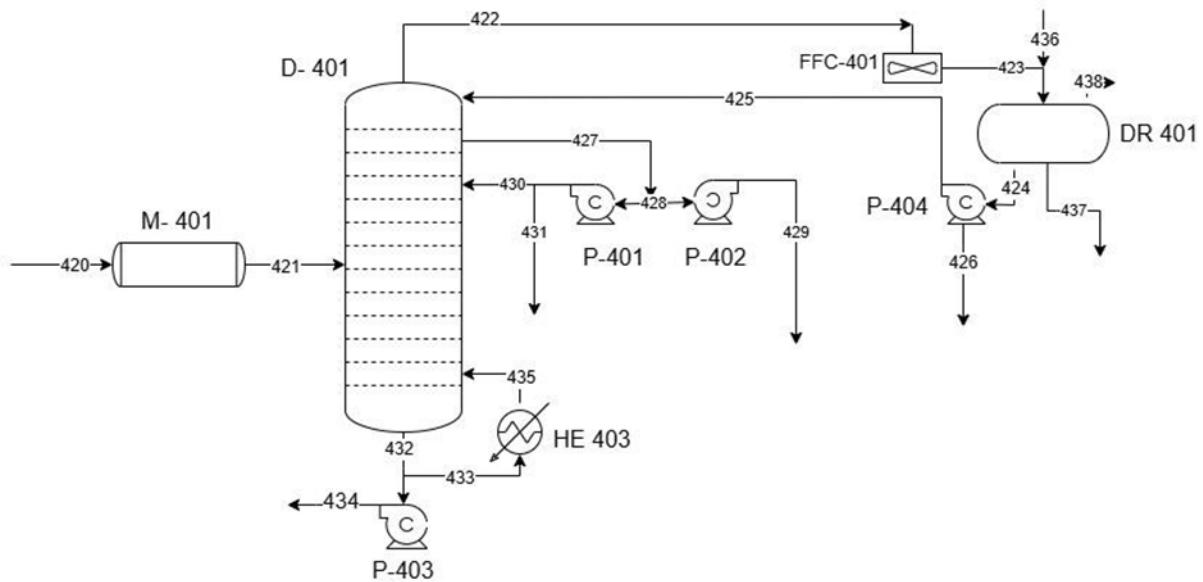


Figure 4.8: Benzene Column

Table 4.5: Stream Data - Benzene Column

Stream No.	Composition
420, 421	Benzene, LAB, Paraffin, Heavy Alkylates
422, 423, 424, 425	Benzene
427, 428, 429, 430, 431	Benzene
432, 433, 434, 435	LAB, Paraffin, Heavy Alkylates, Benzene
436	Makeup Benzene
426	Benzene Drag
437	Wastewater (containing stripped-off impurities)
438	Off Gas (to Flare)

4.4.3 Paraffin Column

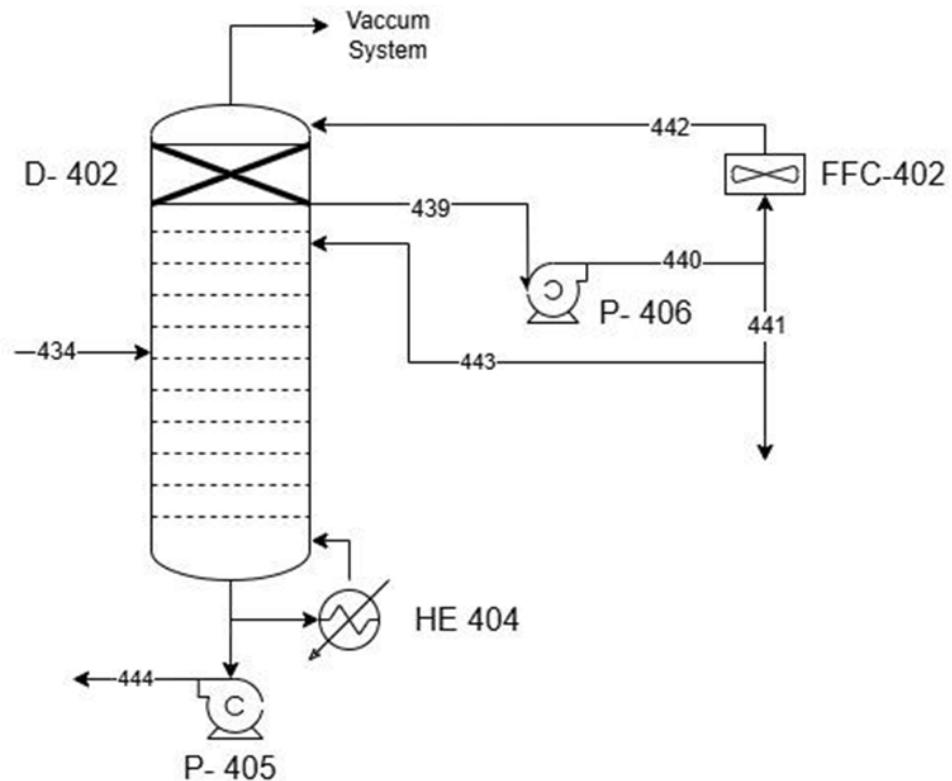


Figure 4.9: Paraffin Column

Table 4.6: Stream Data - Paraffin Column

Stream No.	Composition
434	LAB, Paraffin, Heavy Alkylate, Benzene
439, 440, 441, 442, 443	Paraffin, Benzene
444	LAB, Heavy Alkylates

4.4.4 LAB Column

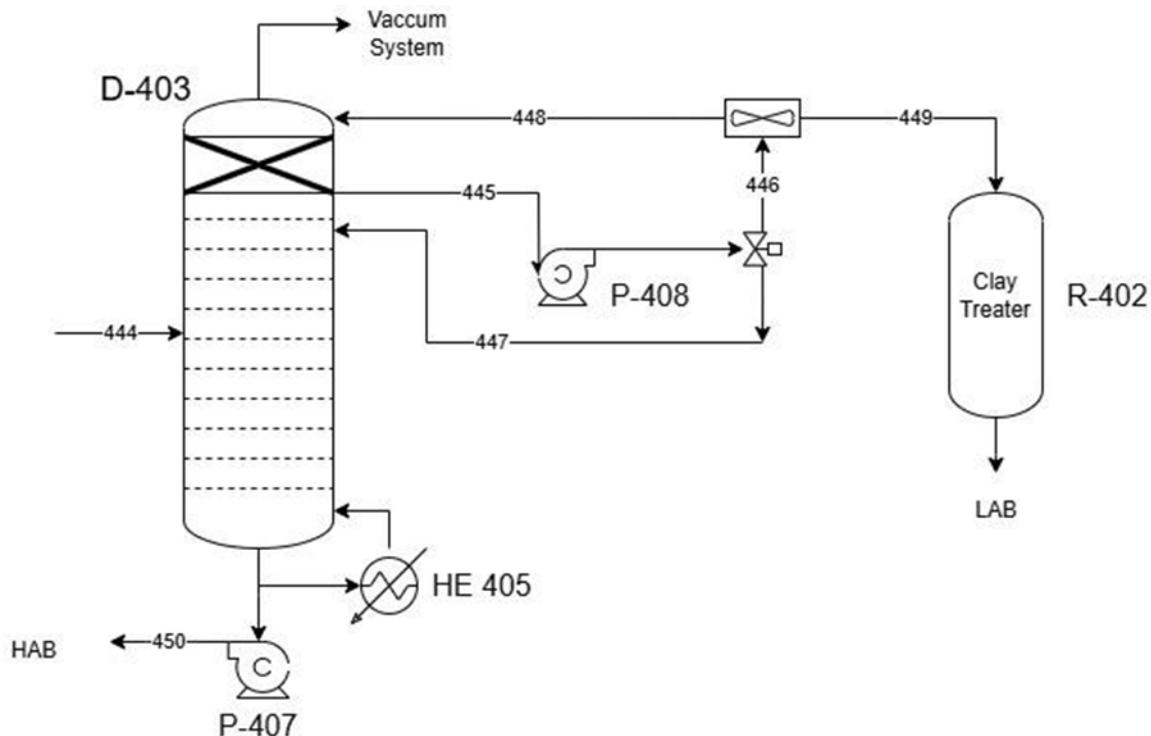


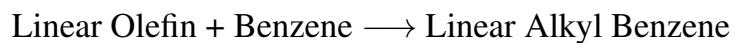
Figure 4.10: LAB column

Table 4.7: Stream Data - LAB Column

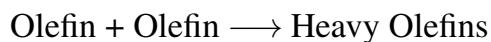
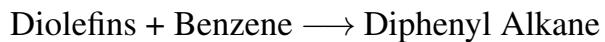
Stream No.	Composition
444	LAB, Heavy Alkyrate
445, 446, 447, 448, 449	LAB
450	Heavy Alkylates

This process is used to alkylate benzene by reacting it with monoolefins coming from PEP unit in the presence of a heterogenous catalyst (zeolite). Primary product formed is Linear Alkyl Benzene whereas heavy alkylates are formed as byproducts.

Main Reaction:



Side Reactions:



These heavy olefins can further react to form heavy alkylates but removal of diolefins in the Define unit and the selectivity of the catalyst ensures that side products are produced in minimal amounts.

Process Flow:

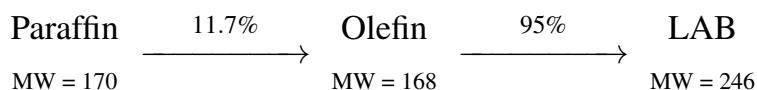
- Feed to Detal unit is C10-C14 paraffin stream containing 10-15% olefins produced upstream in Pacol unit. This incoming feed is mixed with excess of benzene (to enhance selectivity) and fed to Detal reactor wherein reaction occurs to form Linear Alkyl Benzene.(figure 4.7)
- The production of polymer like byproducts hampers the catalyst activity and thus two reactors are used to ensure one of them remains online while the other gets regenerated. The regeneration is done by washing the catalyst with hot benzene to remove the tar like polymers.
- After passing through a fixed bed reactor, the reaction as well as regenerant effluent are passed through the benzene column wherein benzene is separated and recycled back to the Detal reactor.(figure 4.8)
- The bottoms from the benzene column is passed through the paraffin column that separates out paraffin from the mixture and recycles it back to Pacol unit.(figure 4.9)
- The bottoms from paraffin feed is fed in succession to LAB column that separate out the main product Linear Alkyl Benzene and heavy alkylates.(figure 4.10)

Linear Alkyl Benzene is passed through clay treater to remove trace impurities of olefins or aromatics that might increase the Bromine Index.[4]

Chapter 5

Mass Balance

This chapter presents the mass balance for various processes involved in the production of Linear Alkylbenzene (LAB). The calculations are based on a production capacity of **135,000 TPA LAB** with an assumed operation time of **8000 hours per year**. With this information, we back calculated the required amount of reactants on the basis of the below conversions.



For calculation we have applied material balance assuming no accumulation anywhere. We have used conversion data for the reactors(kinetics were used later in simulation) and for the distillation column we had assumed 99% recovery of the light key.

5.1 Pacol Process

Table 5.1: Mass Balance for Pacol Process

Component	Inlet Mass Flow Rate (MT/day)	Outlet Mass Flow Rate (MT/day)
Paraffin	2510	2190
Monoolefin	0	290
Diolefin	0	13
Aromatic	0	10
Light Hydrocarbon	0	5

From table 5.1, it can been seen 13% of paraffin gets converted to mono-olefin, diolefins, aromatics and light hydrocarbons(in 90:3:3:4 molar ratio)

5.2 Define Process

Table 5.2: Mass Balance for Define Process

Component	Inlet Mass Flow Rate (MT/day)	Outlet Mass Flow Rate (MT/day)
Paraffin	2190	2200
Monoolefin	290	300
Diolefin	13	1
Aromatics	10	10
Light Hydrocarbon (in reaction mixture)	5	0
Light Hydrocarbon (separated out)	0	5

In Define process, 90% of the diolefins are converted to mono-olefins and paraffins in 1:1 ratio, while 99% of the lighter hydrocarbons are separated out.(Table 5.2)

5.3 PEP Process

Table 5.3: Mass Balance for PEP Process

Component	Inlet Mass Flow Rate (MT/day)	Outlet Mass Flow Rate (MT/day)
Paraffin	2200	2200
Monoolefin	300	300
Diolefin	1	1
Aromatics (In feed)	10	0
Aromatics (adsorbed and separated)	0	10
Benzene (from Detal)	610	0
Benzene (to Detal)	0	610

5.4 Detal Process

Table 5.4: Mass Balance for Detal Process

Component	Inlet Mass Flow Rate (MT/day)	Outlet Mass Flow Rate (MT/day)
Paraffin	2200	2200
Monoolefin	300	0
Benzene from PEP	610	610
Linear Alkylbenzene (LAB)	0	410
Make-up benzene	140	0
Heavy Alkylate (HAB)	0	25

In Detal process, mono-olefins are converted to Linear Alkyl Benzene and Heavy Alkylates in molar ratio 19:1(Table 5.4).Benzene from PEP process is used for recycling while make up benzene is added for reaction to proceed.

5.5 Benzene Column

Table 5.5: Mass Balance for Benzene Column

Component	Inlet Mass Flow Rate (MT/day)	Outlet Top (MT/day)	Outlet Bottom (MT/day)
Paraffin	2200	0	2200
Benzene	610	604	6
Linear Alkylbenzene (LAB)	410	0	410
Heavy Alkylate (HAB)	25	0	25

We assume 99% recovery of benzene in the benzene column and simple mass balance was applied.(table 5.5)

5.6 Paraffin Column

Table 5.6: Mass Balance for Paraffin Column

Component	Inlet Mass Flow Rate (MT/day)	Outlet Top (MT/day)	Outlet Bottom (MT/day)
Paraffin	2200	2175	25
Benzene	6	6	0
Linear Alkylbenzene (LAB)	410	0	410
Heavy Alkylate (HAB)	25	0	25

We assume 99% recovery of paraffin which can be recycled back to the process.(table 5.6)

5.7 LAB Column

Table 5.7: Mass Balance for LAB Column

Component	Inlet Mass Flow Rate (MT/day)	Outlet Top (MT/day)	Outlet Bottom (MT/day)
Paraffin	25	25	0
Benzene	6	6	0
Linear Alkylbenzene (LAB)	410	405	5
Heavy Alkylate (HAB)	25	0	25

We assume 99% recovery of Linear Alkyl Benzene as an initial guess for mass balance, the exact recovery would be calculated in subsequent stages after completing simulation.(table 5.7)

Chapter 6

Flowsheet Simulation - Aspen Hysys

Aspen HYSYS is the process modeling tool we used to simulate linear alkylbenzene. It is one of the leading packages for process engineering. It allows us to create detailed flow sheets, and study process behavior under different conditions and also in a steady state. It assists in designing and sizing various unit operations like distillation, flash, reactor, etc. With the help of Aspen HYSYS, we can even optimize the process parameters to improve yield, efficiency, and product quality.

We have not considered production of diolefins and aromatics as they are formed in very less quantity($\sim 2\%$ of total paraffin).

6.1 Details of Simulation

6.1.1 Pacol process - Paraffin conversion to Olefin

The first process of LAB production, as shown in figure 6.2, requires feed containing hydrogen and paraffin in a ratio of 5:1 by molar. Here simulation consists of exchanging heat with the feed to increase its temperature i.e., from stream 1 to 2 and then to 2, so that endothermic Dehydrogenation reaction can occur in PFR-101 as seen clearly from the PFD. In the actual process, a radial flow reactor is required, we are using a catalytic conversion reactor to incorporate the kinetics of the reaction. The products from this reaction are separated using flash i.e., in V-100 to separate product olefins and hydrogen streams 8 and 7 respectively. After this hydrogen is recycled using RCY-2.

6.1.2 Detal process - Forming LAB using Benzene and Olefin

Feed pumped through P-100 is mixed with Benzene in MIX-100. Outlet stream 11 is used as feed for the Detal process PFR-101. For this reaction, a catalytic fixed bed reactor is required(figure 6.3). To incorporate the kinetics we are using catalytic conversion reactor PFR-100. The product outlet is then processed to various distillation columns to separate different components. Benzene as an outlet from the top of distillation column T-100 is recycled using RCY-1 to reuse benzene.

6.1.3 Distillation process

The product from Detal reactor is a mixture of linear alkylbenzene, heavy alkylates, paraffin, and benzene. To increase the purity of the product, we require distillation columns(figure 6.4) to separate these compounds in decreasing order of their volatility. Hence, we have used T-100, T-101, and T-102 for separation. T-100 is used to separate benzene for reuse in Detal process. T-101 is used to separate unreacted Paraffins and T-102 is used to separate linear alkylbenzene from heavy alkylated

6.2 Overall Process Flow Diagram

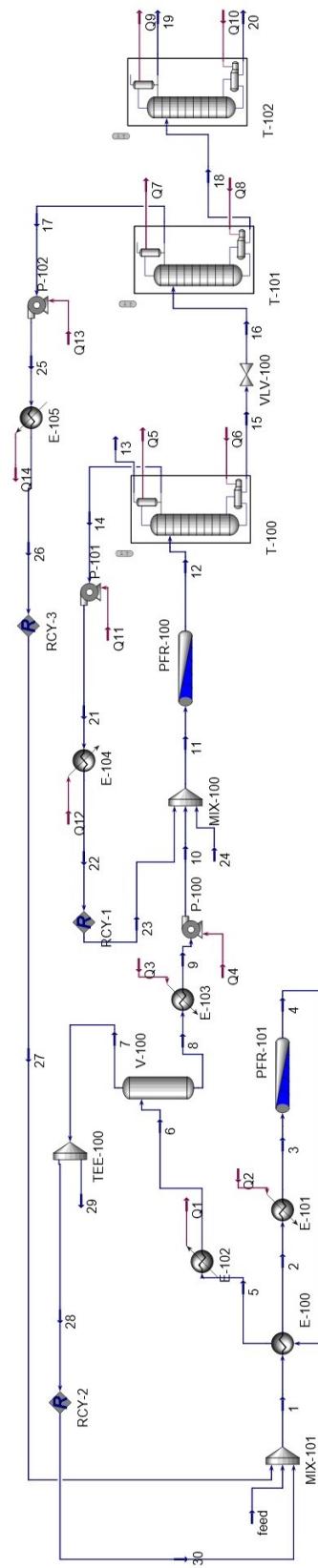


Figure 6.1: Overall Process Flow Diagram

6.2.1 Pacol Process Flow Diagram

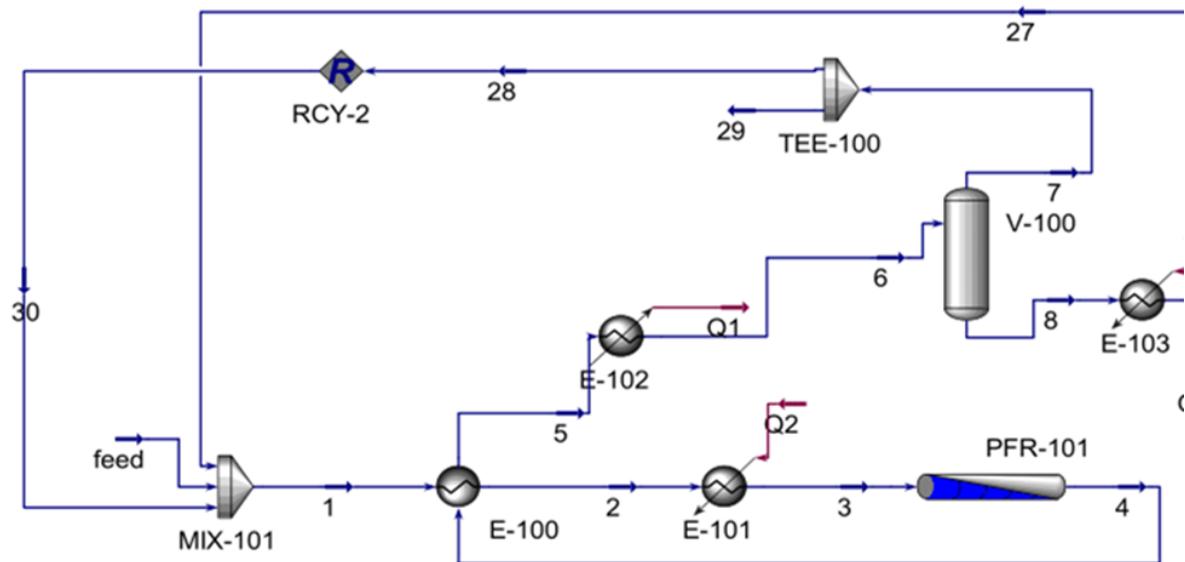


Figure 6.2: Pacol Process Flow Diagram

6.2.2 DETAL Process Flow Diagram

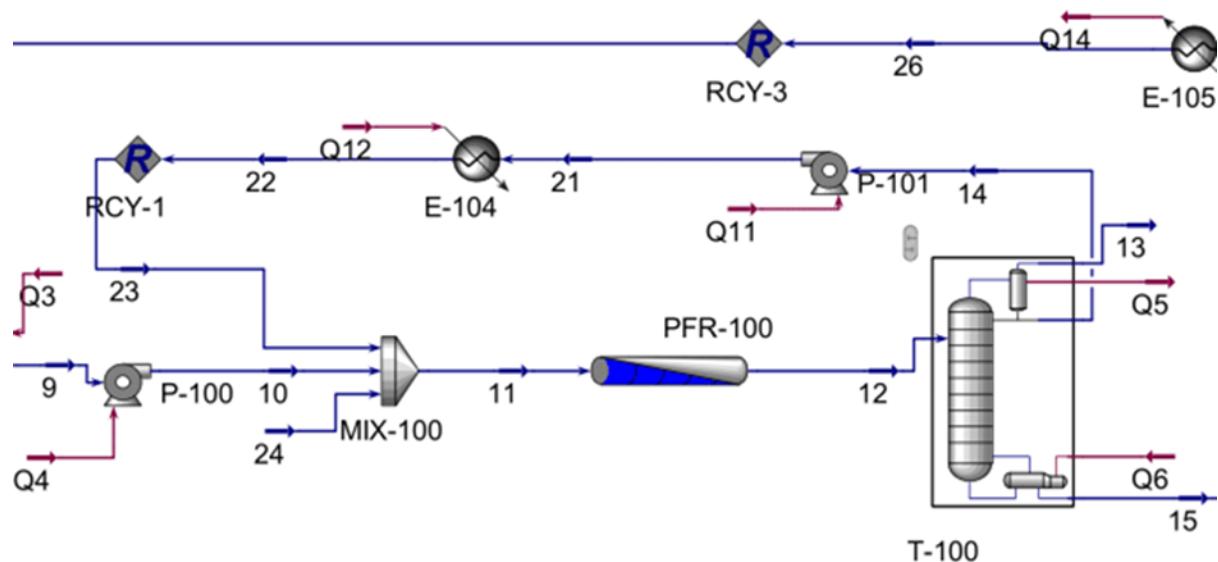


Figure 6.3: DETAL Process Flow Diagram

6.2.3 Distillation Columns

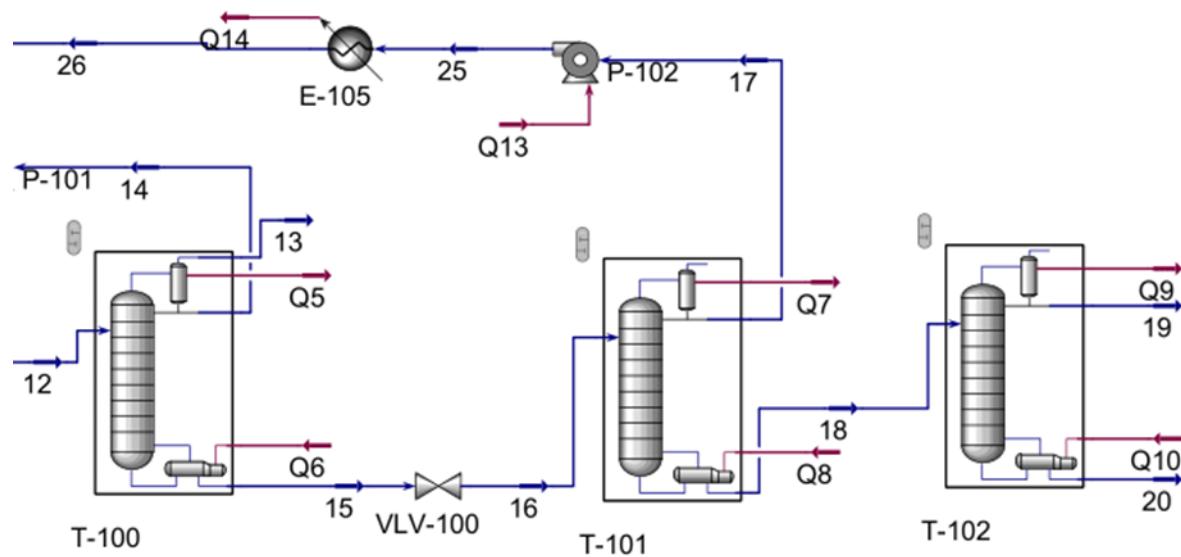


Figure 6.4: Distillation Columns

Table 6.1: Material Streams Process Flow Data

Stream	Units	Feed	1	2	3	4	5
Vapour Fraction	-	0.4959	0.8268	1.0000	1.0000	1.0000	1.0000
Temperature	°C	50.00	49.98	-200.00	450.00	426.50	216.90
Pressure	bar	2.40	2.40	2.40	2.40	2.40	2.40
Molar Flow	mol/sec	40.83	991.39	991.39	991.39	1012.50	1012.50
Mass Flow	kg/sec	3.54	30.92	30.92	30.92	30.92	30.92
Liquid Volume Flow	lit/sec	5.25	62.64	62.64	62.64	63.11	63.11
Heat Flow	MW	-6.98	-57.86	-35.56	-9.01	-9.01	-31.31
Stream	Units	6	7	8	9	10	
Vapour Fraction	-	0.8303	1.0000	0.0000	0.0000	0.0000	
Temperature	°C	50.05	50.00	50.00	75.00	75.02	
Pressure	bar	2.40	2.40	2.40	2.40	3.00	
Molar Flow	mol/sec	1012.50	840.28	171.69	171.69	171.69	
Mass Flow	kg/sec	30.92	1.78	29.14	29.14	29.14	
Liquid Volume Flow	lit/sec	63.11	24.35	38.75	38.75	38.75	
Heat Flow	MW	-55.28	0.46	-55.75	-54.11	-54.11	
Stream	Units	11	12	13	14	15	
Vapour Fraction	-	0.0000	0.0141	1.0000	0.0000	0.0000	
Temperature	°C	73.63	133.90	74.46	74.46	273.10	
Pressure	bar	3.00	3.00	2.00	2.00	3.00	
Molar Flow	mol/sec	472.78	452.78	0.53	281.11	171.03	
Mass Flow	kg/sec	52.67	52.67	0.018	21.95	30.69	
Liquid Volume Flow	lit/sec	65.42	64.97	0.029	24.88	40.06	
Heat Flow	MW	-36.64	-36.64	0.02	15.87	-43.75	
Stream	Units	16	17	18	19	20	
Vapour Fraction	-	0.7796	0.0000	0.0000	0.0000	0.0000	
Temperature	°C	206.10	95.85	253.90	182.80	240.60	
Pressure	bar	0.50	0.02	0.20	0.02	0.10	
Molar Flow	mol/sec	171.03	150.83	20.20	18.89	1.31	
Mass Flow	kg/sec	30.69	25.68	5.01	4.65	0.36	
Liquid Volume Flow	lit/sec	40.06	34.19	5.88	5.44	0.44	
Heat Flow	MW	-43.75	-48.61	-8.00	-8.40	-0.51	
Stream	Units	21	22	23	24	25	
Vapour Fraction	-	0.0000	0.0000	0.0000	0.0000	0.0000	
Temperature	°C	74.51	90.00	90.00	20.00	95.93	
Pressure	bar	3.00	3.00	3.00	3.00	2.40	
Molar Flow	mol/sec	281.11	281.11	281.11	20.00	150.83	
Mass Flow	kg/sec	21.95	21.95	21.95	1.56	25.68	
Liquid Volume Flow	lit/sec	24.88	24.88	24.88	1.77	34.19	
Heat Flow	MW	15.87	16.48	16.48	0.99	-48.61	
Stream	Units	26	27	28	29	30	
Vapour Fraction	-	0.0000	0.0000	1.0000	1.0000	1.0000	
Temperature	°C	50.00	50.00	50.00	50.00	50.00	
Pressure	bar	2.40	2.40	2.40	2.40	2.40	
Molar Flow	mol/sec	150.83	150.83	803.33	36.97	799.72	
Mass Flow	kg/sec	25.68	25.69	1.70	0.078	1.69	
Liquid Volume Flow	lit/sec	34.19	34.19	23.28	1.07	23.18	
Heat Flow	MW	-51.28	-51.31	0.44	0.02	0.44	

Table 6.2: Stream Composition Data (Mole Fraction)

Component	Stream Number										
	Feed	1	2	3	4	5	6	7	8	9	10
Hydrogen	0.4966	0.8266	0.8266	0.8266	0.8302	0.8302	0.8302	0.9994	0.0019	0.0019	0.0019
n-C12	0.5034	0.1733	0.1733	0.1733	0.1495	0.1495	0.1495	0.0005	0.8783	0.8783	0.8783
1-C24=	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
3-LAB*	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Benzene	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
1-Dodecene	0.0000	0.0001	0.0001	0.0001	0.0204	0.0204	0.0204	0.0001	0.1198	0.1198	0.1198
2-LAB*	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Component	Stream Number									
	11	12	13	14	15	16	17	18	19	20
Hydrogen	0.0009	0.0009	0.5676	0.0005	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
n-C12	0.3189	0.3331	0.0000	0.0000	0.8817	0.8817	0.9993	0.0036	0.0039	0.0000
1-C24=	0.0000	0.0010	0.0000	0.0000	0.0026	0.0026	0.0000	0.0217	0.0002	0.3306
3-LAB*	0.0000	0.0240	0.0000	0.0000	0.0634	0.0634	0.0000	0.5370	0.5487	0.3688
Benzene	0.6367	0.6215	0.4324	0.9995	0.0006	0.0006	0.0007	0.0000	0.0000	0.0000
1-Dodecene	0.0435	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
2-LAB*	0.0000	0.0195	0.0000	0.0000	0.0517	0.0517	0.0000	0.4377	0.4473	0.3006

Component	Stream Number									
	21	22	23	24	25	26	27	28	29	30
Hydrogen	0.0005	0.0005	0.0004	0.0000	0.0000	0.0000	0.0000	0.9994	0.9994	0.9994
n-C12	0.0000	0.0000	0.0000	0.0000	0.9993	0.9993	1.0000	0.0005	0.0005	0.0005
1-C24=	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
3-LAB*	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Benzene	0.9995	0.9995	0.9996	1.0000	0.0007	0.0007	0.0000	0.0000	0.0000	0.0000
1-Dodecene	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0001	0.0001
2-LAB*	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Where:

LAB = Linear Alkyl Benzene

n-C12 = Paraffin

1-Dodecene = Olefin

n-C24 = Heavy Alkylate

6.3 Modification for Equipment Used in PFD and Simulation

Table 6.3: Equipment Modifications

Equipment code	Actual PFD Equipment	Equipment in Simulation
PFR-101	Radial flow reactor	Plug Flow Reactor
PFR-100	Catalytic fixed bed reactor	Plug Flow Reactor

6.4 Comparison of Mass Balance and Simulation Results

We are enlisting the results we got in Chapter 5 along with the simulation results to compare them. These values are obtained by linear mass balance.

6.4.1 Pacol Process

Table 6.4: Mass balance Comparison-Pacol process

Component	Manual		Simulation	
	Inlet (ton/hr)	Outlet (ton/hr)	Inlet (ton/hr)	Outlet (ton/hr)
N-Paraffin	104.53	91.28	105.36	92.47
Mono Olefin	0	12.13	0	12.46
Hydrogen	0	0.39	5.95	6.09

6.4.2 Detal Process

Table 6.5: Mass balance Comparison-Detal process

Component	Manual		Simulation	
	Inlet (ton/hr)	Outlet (ton/hr)	Inlet (ton/hr)	Outlet (ton/hr)
N-Paraffin	91.53	91.53	92.47	92.47
Mono Olefin	12.38	0	12.46	0
Hydrogen	0	0	0	0
Benzene	31.12	25.44	84.64	79.10
LAB	0	17.02	0	17.47
HAB	0	1.04	0	0.53

6.4.3 Benzene Column

Table 6.6: Mass balance Comparison-Benzene Column

Component	Manual			Simulation		
	Inlet (ton/hr)	Outlet at top (ton/hr)	Outlet at bottom (ton/hr)	Inlet (ton/hr)	Outlet at top (ton/hr)	Outlet at bottom (ton/hr)
N-Paraffin	91.53	0	91.53	92.47	0	92.47
Mono Olefin	0	0	0	0	0	0
Hydrogen	0	0	0	0	0	0
Benzene	25.44	25.18	0.25	79.10	79.00	0.03
LAB	17.02	0	17.02	17.47	0	17.47
HAB	1.04	0	1.04	0.53	0	0.53

6.4.4 Paraffin Column

Table 6.7: Mass balance Comparison-Paraffin Column

Component	Manual			Simulation		
	Inlet (ton/hr)	Outlet at top (ton/hr)	Outlet at bottom (ton/hr)	Inlet (ton/hr)	Outlet at top (ton/hr)	Outlet at bottom (ton/hr)
N-Paraffin	91.53	90.62	0.91	92.47	92.42	0.05
Mono Olefin	0	0	0	0	0	0
Hydrogen	0	0	0	0	0	0
Benzene	0.25	0.25	0	0.03	0.03	0
LAB	17.02	0	17.02	17.47	0	17.47
HAB	1.04	0	1.04	0.53	0	0.53

6.4.5 LAB Column

Table 6.8: Mass balance Comparison-LAB Column

Component	Manual			Simulation		
	Inlet (ton/hr)	Outlet at top (ton/hr)	Outlet at bottom (ton/hr)	Inlet (ton/hr)	Outlet at top (ton/hr)	Outlet at bottom (ton/hr)
N-Paraffin	0.91	0.91	0	0.05	0.05	0
Mono Olefin	0	0	0	0	0	0
Hydrogen	0	0	0	0	0	0
Benzene	0	0	0	0	0	0
LAB	17.02	16.84	0.17	17.47	16.70	0.78
HAB	1.04	0	1.04	0.53	0	0.53

Chapter 7

Sensitivity Analysis

7.1 Pacol Reactor

The kinetics of the dehydrogenation reaction is [8]:

$$R = \frac{k'_p K_p P_p}{DEN} \quad (7.1)$$

$$DEN = 1 + (K_H P_{H_2})^{0.5} \quad (7.2)$$

Where value of k'_p , K_p , P_p , K_H , P_{H_2} are given in reference.

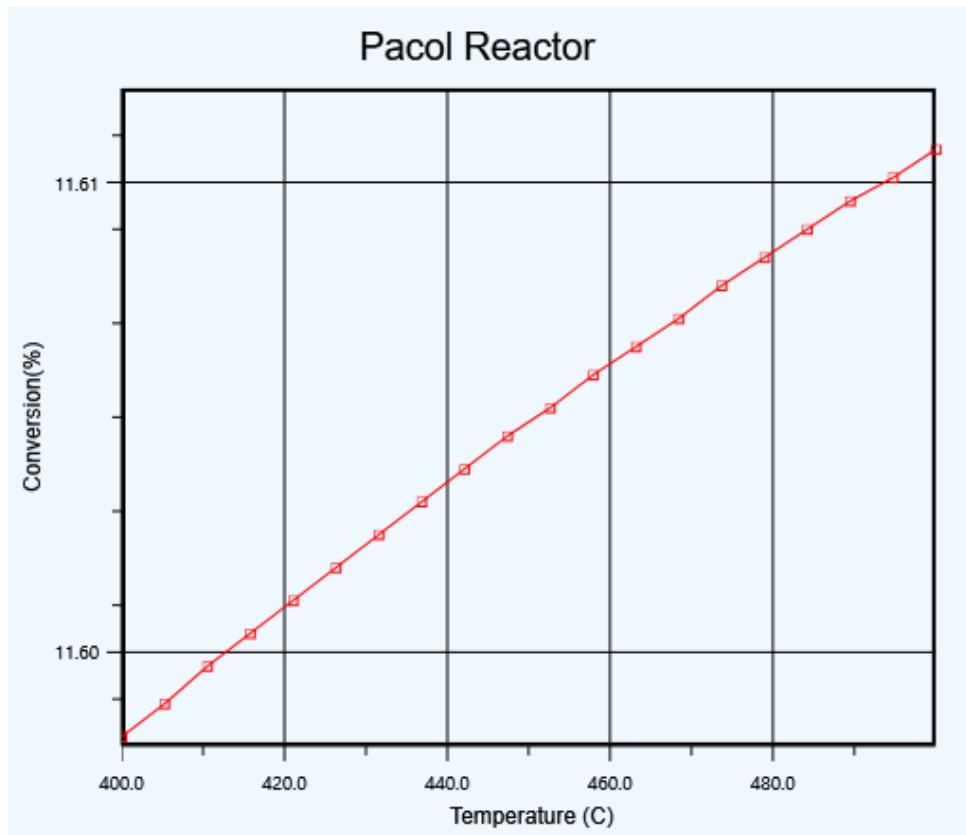


Figure 7.1: Conversion vs Temperature for Pacol Reactor

After doing sensitivity analysis as shown in Figure 7.1, we see there is not a strong relation between temperature and the conversion achieved. We know the catalyst being

used has good activity in the range 450-480°C. So, we would send the feed at 450°C wherein we get required conversion as well catalyst activity is not affected much.

7.2 Datal Reactor

The kinetics are first order with respect to benzene and 1-dodecene [7].

$$R_{2-LAB} = 402.783 \exp\left(\frac{-45730}{RT}\right) C_B C_{1-D} \quad (7.3)$$

$$R_{3-LAB} = 743.969 \exp\left(\frac{-46640}{RT}\right) C_B C_{1-D} \quad (7.4)$$

Where C_B and C_{1-D} refer to concentration of benzene and 1-dodecene.

Table 7.1: Effect of Temperature on LAB Production

Temperature	2-LAB(%)	3-LAB(%)	HAB(%)	Total Conversion
60	43.05	52.23	4.72	100
66.67	43.03	52.46	4.51	100
73.33	43	52.69	4.31	100
80	42.97	52.9	4.10	99.97
86.67	42.9	53.06	3.89	99.85
93.33	42.76	53.11	3.70	99.57
100	42.47	52.96	3.54	98.97
106.7	42.04	52.62	3.42	98.08
113.3	41.51	52.14	3.33	96.98
120	40.78	51.38	3.34	95.50

The analysis, as shown in Table 7.1 reveals that the overall conversion reduces with increasing temperature. So we would prefer temperatures in the range of 65-75°C . As seen in Figure 7.2, we see similar increase in 2-LAB and 3-LAB with increasing temperatures so choosing higher temperature does not ensure a better selectivity towards 2-LAB.

We have not done proper equipment sizing but we see a sudden spike in conversion after a volume of 200 m³, as seen in Figure 7.3 so we should definitely size the reactor having volume greater than 200 m³.

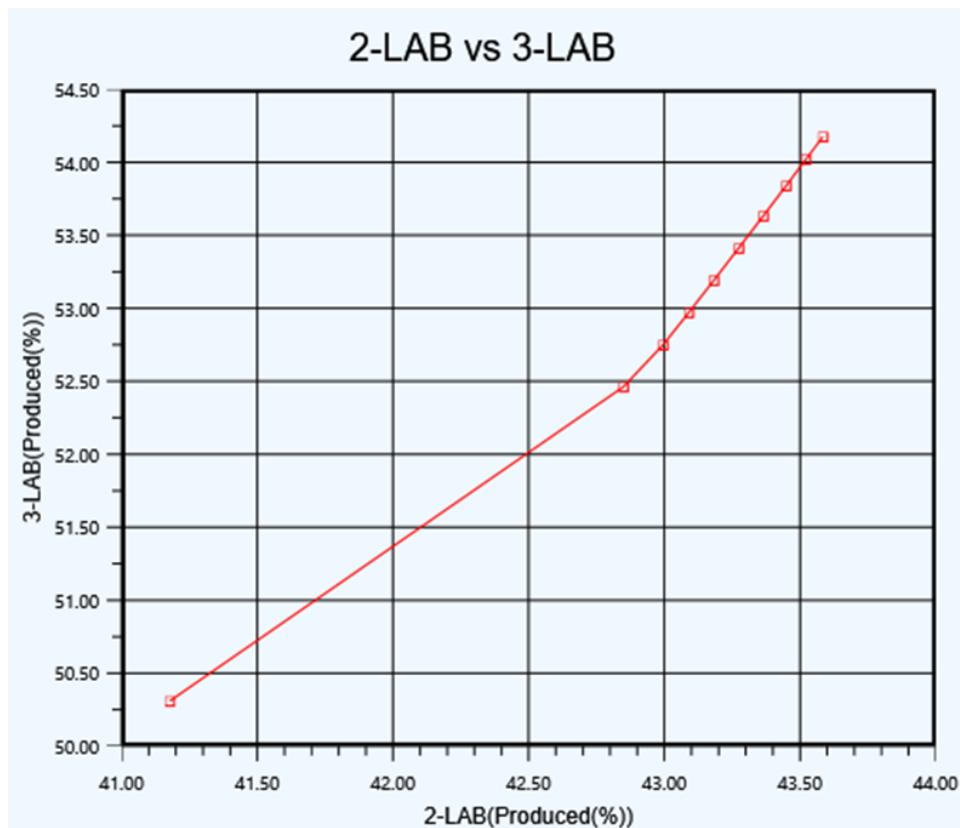


Figure 7.2: 2-LAB vs 3-LAB production %

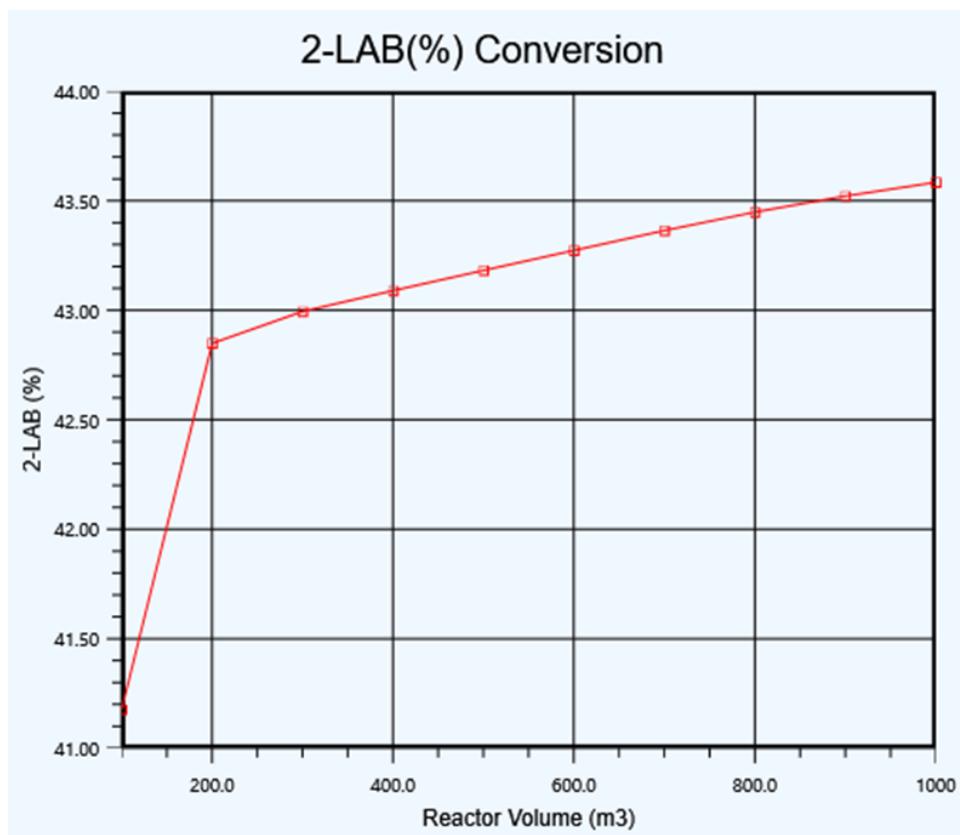


Figure 7.3: 2-LAB vs Volume of Reactor

7.3 Benzene and Paraffin Column

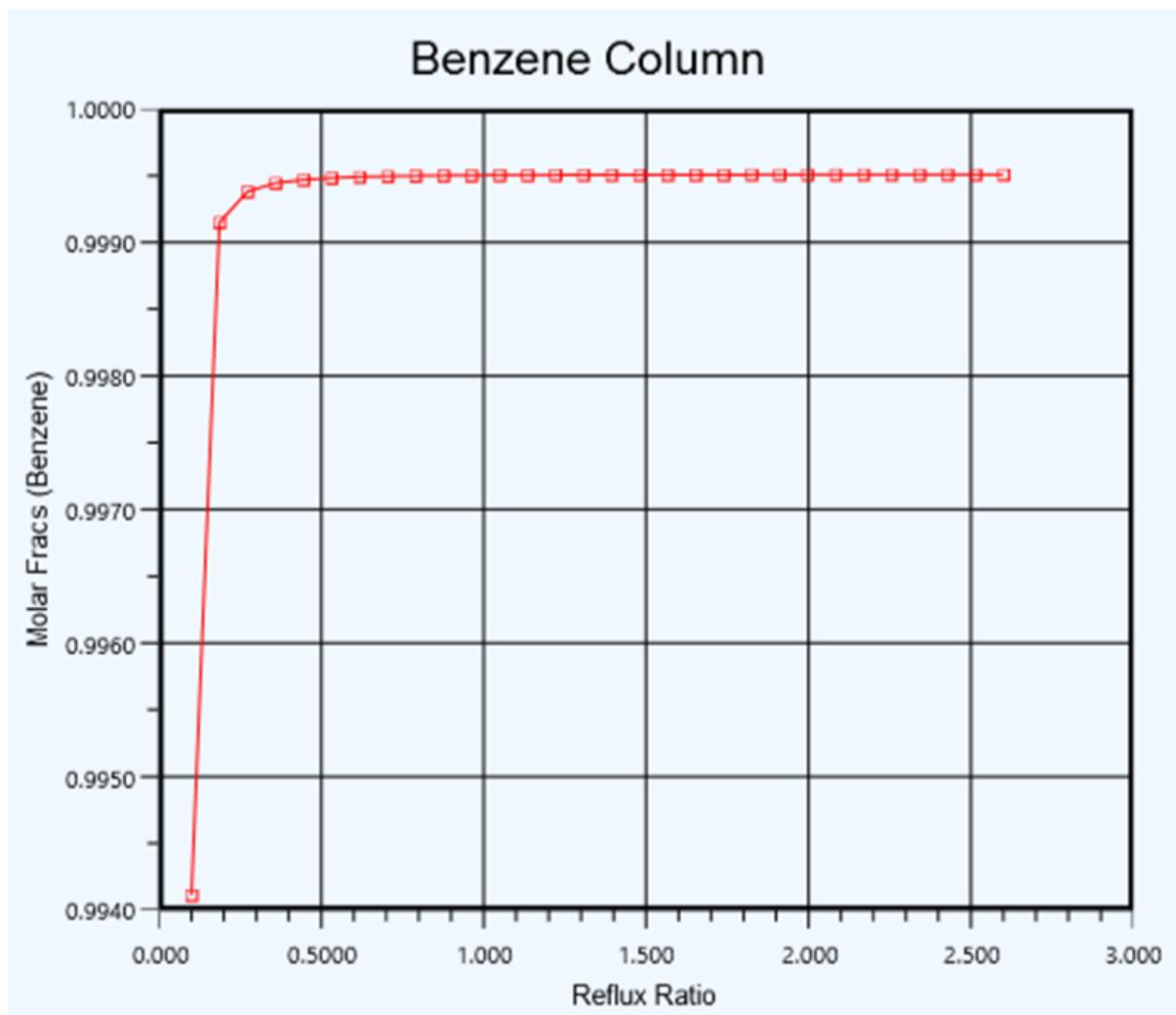


Figure 7.4: Molar recovery of Benzene at top vs Reflux Ratio

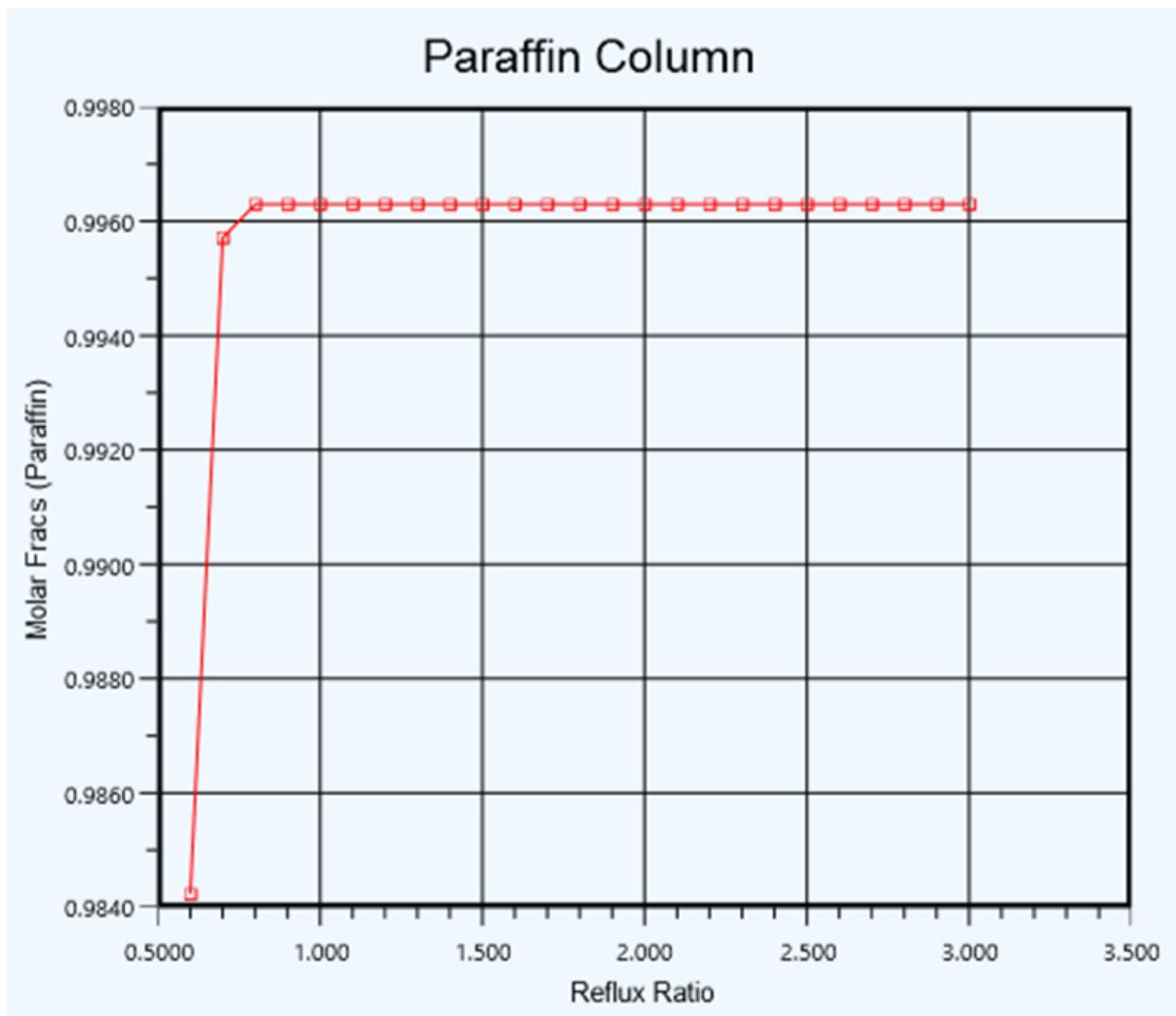


Figure 7.5: Molar recovery of Paraffin at top vs Reflux Ratio

These are the separation columns that are used to separate out reactants and products. The analysis conducted helped us obtain optimal reflux ratio such that we can separate out reactants and recycle them back to the reactor. Both graphs showed a similar trend wherein the recovery of product from overhead became stagnant after a certain point, as shown in Figure 7.4 and Figure 7.5 .

7.4 LAB Column

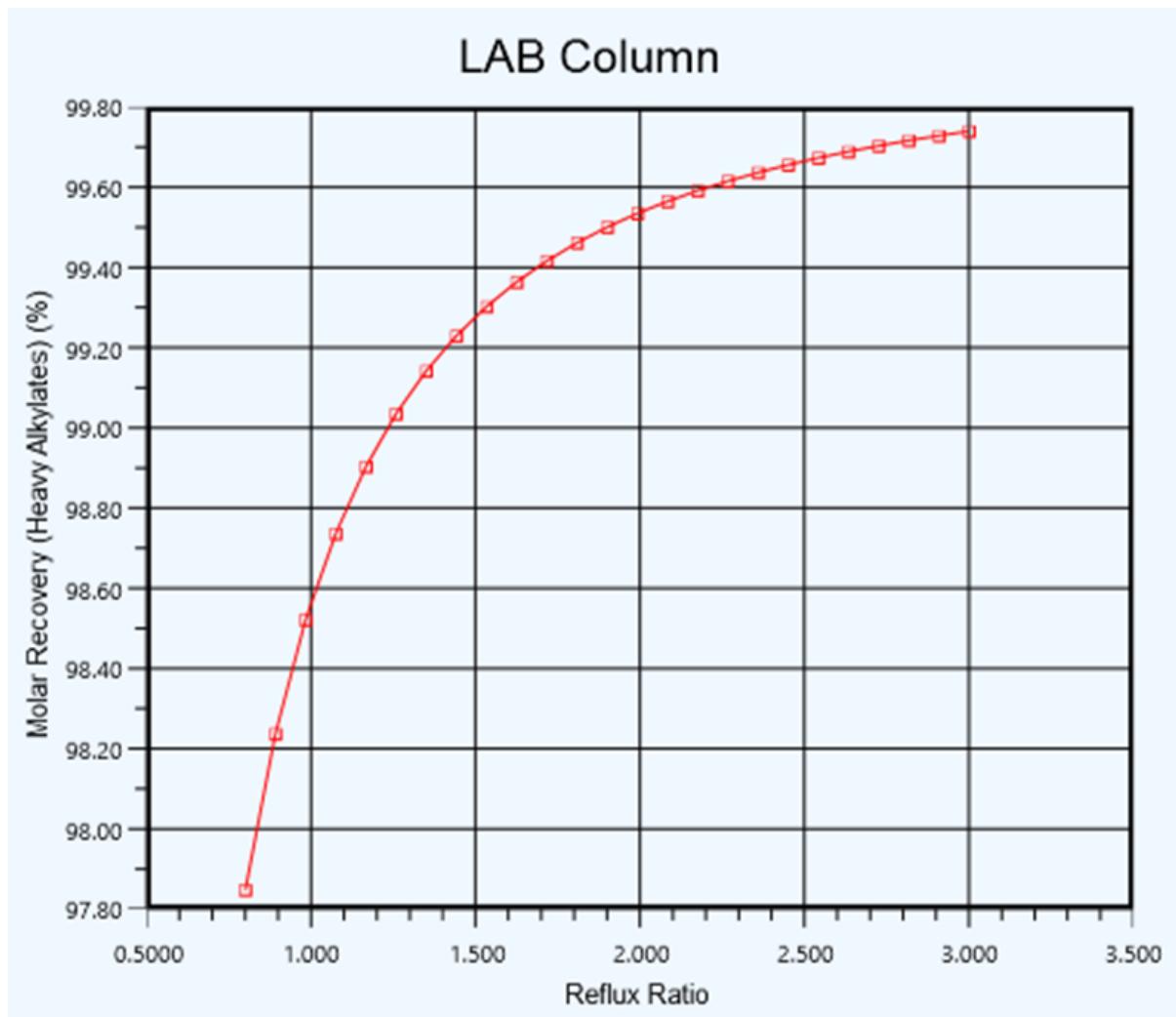


Figure 7.6: Molar recovery of Heavy Alkylate at bottom vs Reflux ratio

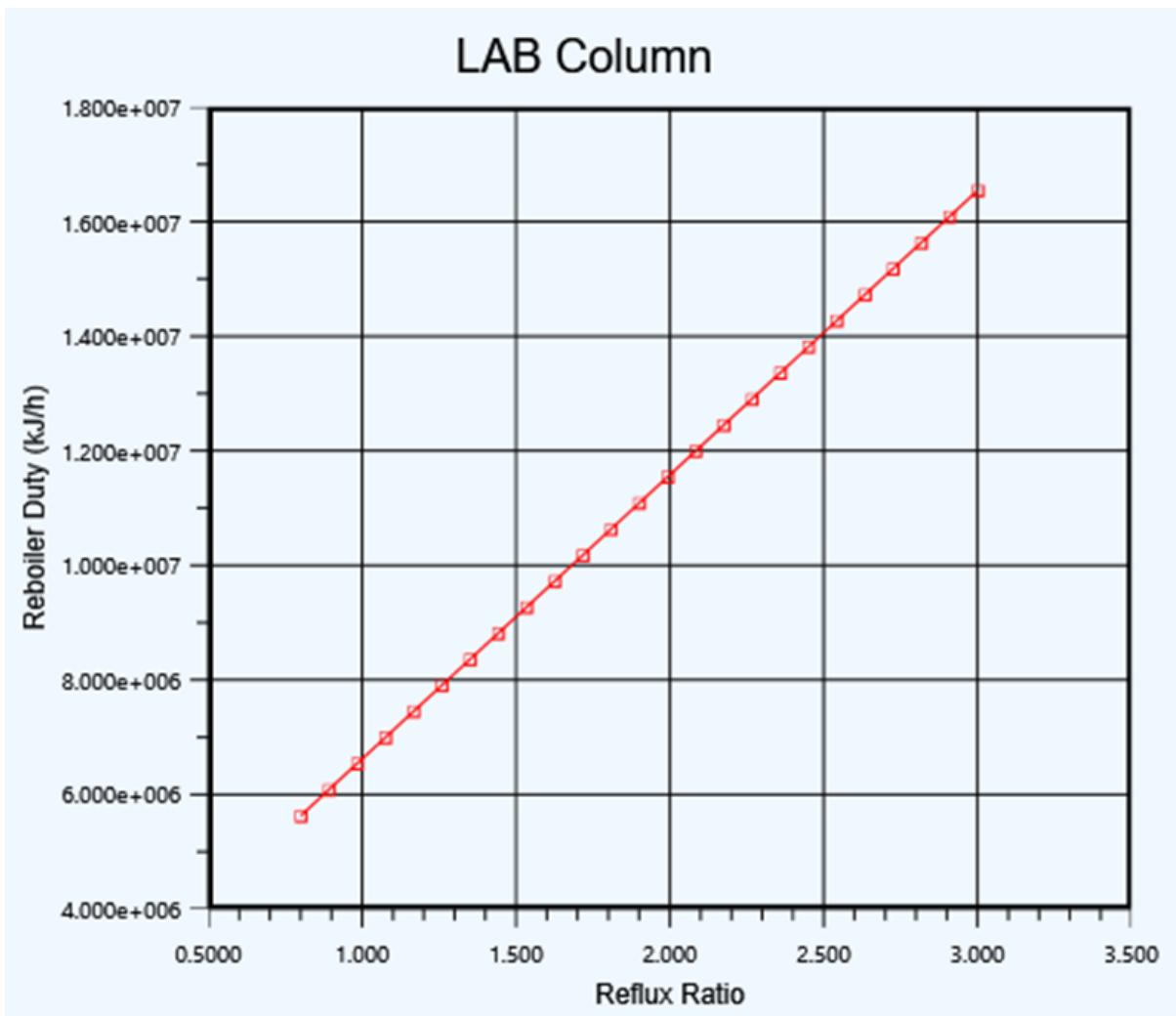


Figure 7.7: Reboiler Duty vs Reflux Ratio

Sensitivity Analysis was conducted to find the optimal reflux ratio. As shown in Figure 7.6 and Figure 7.7, it was found that upon increasing reflux ratio the separation increased but so did reboiler duty. It is a tradeoff between purity and reboiler duty. The reboiler duty depends on the expected purity of the product. For now, we have chosen 1.5 as optimal reflux ratio.

Chapter 8

Equipment sizing and Costing

This chapter describes the sizing and costing of various major equipment required for linear alkylbenzene production. The equipment costs have been scaled to the cost as of 2002. The calculation done in this chapter forms the basis for the final cost calculation in 2024. Equipment costs have been estimated using Nomograms from Peters et. al and Walas et. al.[10]

8.1 Pumps

As per our plant design, we require three pumps (P-100, P-101, P-102). These are single-stage centrifugal pumps with a standard rpm of 3500 (high-speed rotation). Since the flow rates are high and the pressure head is moderate, pumps of high speed, i.e., 3500 rpm, are recommended.

Formula for calculation:

$$W = \frac{\Delta P}{\rho} + g\Delta z + \frac{\Delta P_f}{\rho} \quad (8.1)$$

$$P = \frac{W \cdot m}{\eta_p} \quad (8.2)$$

$$F = \frac{-\Delta P_f}{\rho} = \frac{2fV^2L}{g_c \cdot D} \quad (8.3)$$

$$f = \frac{0.046}{(N_{Re})^{0.2}} \quad (8.4)$$

where,

W = work done by pump (J/kg)

ΔP = difference in pressure = $P_2 - P_1$ (N/m²)

Δz = difference in elevation = $z_2 - z_1$ (m)

ΔP_f = pressure drop due to friction in pipe fittings (N/m²)

ρ = density of liquid (kg/m³)

g = acceleration due to gravity (m²/s)

m = mass flow rate (kg/s)

η_p = pump efficiency

P = power required (W)

$\Delta P_f / \rho$ = frictional loss

f = friction factor

V = fluid velocity

L = pipe length

g_c = gravitational constant

D = pipe diameter

N_{Re} = Reynolds number

The calculation for pump P-100 is given below:

$$\Delta P = 6000000 \text{ N/m}^2$$

$$\Delta z = 0$$

$$\rho = 752 \text{ kg/m}^3$$

$\eta_p = 0.8$ (Pump efficiency is based on pump capacity and head, Tower et. al)

$$W = 90.46 \text{ kJ/hr}$$

$$\Delta P_f = 4401 \text{ N/m}^2$$

$$P = 3287 \text{ W}$$

Based on the power requirement, motor efficiency = 80% as per motor efficiency equation given in Peter et. al.[9]

Table 8.1: Pump power calculation

Equipment	Type	P_{in} (bar)	P_{out} (bar)	Head (m)	Mass flow (kg/s)	Flow rate (m ³ /h)	W (J/kg)	Power (W)
P-100	Centrifugal	240	300	9.22	29.14	139.5	90.46	3287
P-101	Centrifugal	200	300	12.80	21.94	89.58	125.65	3581
P-102	Centrifugal	2	240	35.83	25.68	123.1	351.49	11770

8.1.1 Cost Estimation for Pump

The cost estimation of centrifugal pumps is performed using the empirical equations provided by *Walas et al*[10]. The pump cost C is first calculated in **1984 dollars** and then scaled to **2002 dollars** using the **Chemical Engineering Plant Cost Index (CEPCI)**:

$$\text{CEPCI}_{1984} = 322.7, \quad \text{CEPCI}_{2002} = 309.4$$

The cost of a centrifugal pump is estimated using the following equation:

$$C = F_M F_T C_b \quad (8.5)$$

where:

- C = Estimated pump cost (\$) in 1984
- F_M = Material of Construction (MoC) correction factor
- F_T = Type correction factor (for pump configuration)
- C_b = Base cost of the pump

Base Cost Estimation

The base cost of the pump, C_b , is calculated using the following empirical equation:

$$C_b = 1.55 \times \exp \left(8.833 - 0.6019 \ln(Q\sqrt{H}) + 0.0519(\ln(Q\sqrt{H}))^2 \right) \quad (8.6)$$

where:

- Q = Flow rate (gallons per minute, gpm)
- H = Head (feet, ft)

The correction factor for pump configuration, F_T , is determined using:

$$F_T = \exp \left(b_1 + b_2 \ln(Q\sqrt{H}) + b_3(\ln(Q\sqrt{H}))^2 \right) \quad (8.7)$$

For a centrifugal pump operating at 3500 rpm, the empirical coefficients used are:

$$b_1 = 0.0632, \quad b_2 = 0.2744, \quad b_3 = -0.0253$$

Material of Construction (MoC) Factor

For Carbon Steel, the correction factor is given as:

$$F_M = 1.35$$

Final Cost Calculation for 2002

The final pump cost in **2002 dollars** is obtained by scaling the estimated cost using the CEPCI index as follows:

$$C_{2002} = C_{1984} \times \left(\frac{\text{CEPCI}_{2002}}{\text{CEPCI}_{1984}} \right) \quad (8.8)$$

Based on the above equations, the estimated pump costs (\$) for the year **2002** are summarized in Table 8.2.

Table 8.2: Cost for Pumps

Pump	MoC	Process Fluid	Power (W)	Capacity (gallons/min)	C_b	F_t	Cost (\$) 1990	Cost (\$) 2002
P-100	CS	n-C12, 1-Dodecene	3287	614.2	2438.3	1.87	4600	10000
P-101	CS	Benzene	3581	394.4	2301.2	1.94	6026	13100
P-102	CS	n-C12	11770	541.8	2584	1.71	5980	13000

8.2 Reactor

8.2.1 DetaI Reactor

As per our requirement, since this reaction is exothermic, output heat from this reaction is being used as heaters and heat exchangers. For this, an adiabatic reactor is used.

The adiabatic equation for energy balance:

$$\frac{dT}{dV} = \frac{Ua(T_a - T) + \sum_{i=1}^q (-r_{ij})[-\Delta H_{Rx,ij}(T)]}{\sum_{j=1}^m F_j C_{pj}} \quad (8.9)$$

The material balance equation for species A in a **Plug Flow Reactor** is:

$$\frac{dF_A}{dV} = r_{1A} + r_{2A} \quad (8.10)$$

Kirchhoff's Equation for Heat of Reaction

$$H(T_2) = H(T_1) + \int_{T_1}^{T_2} C_p dT \quad (8.11)$$

$$\Delta H(T_2) = \Delta H(T_1) + \int_{T_1}^{T_2} \Delta C_p dT \quad (8.12)$$

Heat Capacity at Constant Pressure

The heat capacity at constant pressure is expressed as a polynomial function of temperature:

$$C_P = a + bT + cT^2 + dT^3 \quad (8.13)$$

where:

- U = Heat transfer coefficient
- r_{ij} = Rate of reaction
- ΔH_r = Heat of reaction
- F = Flow rate
- C_p = Heat capacity
- $\Delta H(T)$ = Heat of reaction at temperature T
- a, b, c, d = constants

Thickness Calculation Based on ASME Code

The thickness of a component, as per Hoop's stress formula from the ASME Code, is given by:

$$t_R = \frac{PD_0}{2(S_aE + 0.4P)} \quad (8.14)$$

After accounting for corrosion and milling, the final thickness is:

$$t = \frac{t_R + c}{1 - \frac{m}{100}} \quad (8.15)$$

where:

- c = Corrosion tolerance
- m = Milling tolerance
- P = Internal pressure
- D_0 = Internal diameter
- S_a = Allowable stress = 140 MPa
- E = Weld efficiency = 0.85
- t_R = Thickness obtained from Hoop's formula
- c = Corrosion allowance = 9 mm
- m = Percentage thinning due to milling = 10

Table 8.3: PFR-100 (Detal Reactor) Parameters

Specifications	Value
Mass flow rate (kg/hr)	189600
Volumetric flow rate (m ³ /hr)	235.5
Residence time (hr)	1.02
Total volume (m ³)	240
Length (m)	19.69
Diameter (m)	3.93
Thickness (mm)	15.5

For cost estimation(figure 8.1), nomograms from Peters et. al[9] have been used. The following are the results for the reactor cost estimation as of Jan 2002 according to the specifications of the Detal reactor(Table 8.3). The purchased cost of jacketed and plug flow reactor are used in the estimation.

Cost (Jan 2002) = \$ 90000 (as estimated from nomogram by Peters et. al[9])(figure 8.1)

8.2.2 Pacol Reactor

Similar calculation is done for Pacol reaction (PFR-101). Volume for the desired conversion is 4 m³. Length and Diameter is calculated by taking ratio of their length as 5:1.

For cost estimation(figure 8.1), nomograms from Peters et. al[9] have been used. The following are the results for the reactor cost estimation as of Jan 2002 based on the specifications for Pacol reactor(Table 8.4). The purchased cost of jacketed and plug flow reactor are used in the estimation.

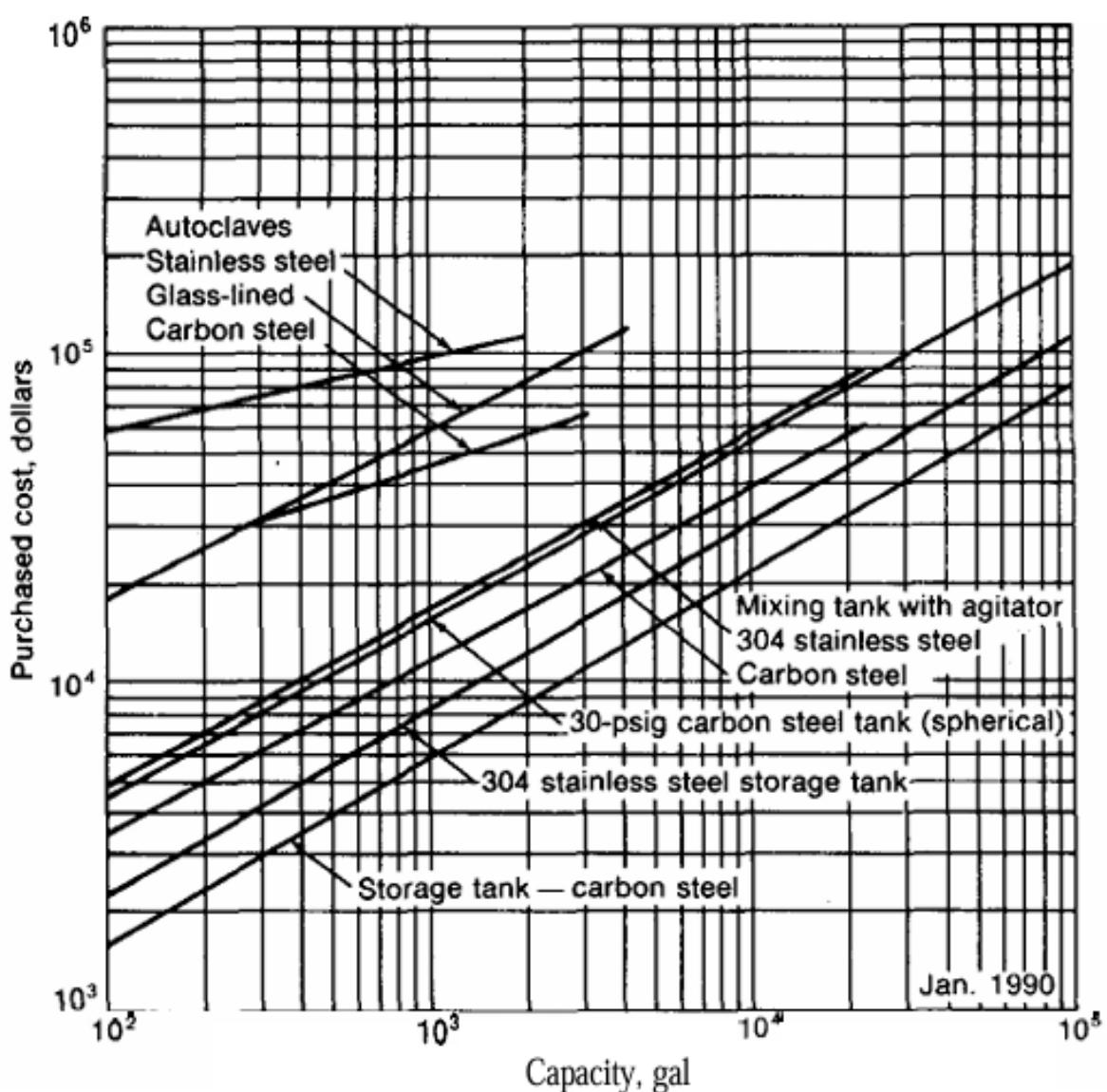


Figure 8.1: Cost of Mixing, storage and pressure tanks

Table 8.4: PFR-101(Pacol Reactor) Parameters

Specifications	Value
Mass flow rate (kg/hr)	111300
Volumetric flow rate (m ³ /hr)	225.5
Residence time (hr)	0.02
Total volume (m ³)	4
Length (m)	5
Diameter (m)	1
Thickness (mm)	9

Cost (Jan 2002) = \$ 18000 (as estimated from nomogram by Peters et. al[9])(figure 8.1)

8.3 Flash Column

For the design of flash columns, correlations from Walas et. al[10] have been used. Flash (V-100) is required after the Pacol process to separate Hydrogen from a mixture of Hydrogen and Paraffin.

The maximum allowable vapor velocity is calculated by using the Souders-Brown equation. The design parameter K , in the Souders-Brown equation is an empirical parameter and is a key factor for the sizing of the gas-liquid separators vessel diameter. It is a function of pressure and fluid properties. The density of liquid and vapor and the vapor flow rate are found using the ASPEN HYSyS Simulation.

$$K = 0.35 - 0.01 \cdot \frac{\text{Design pressure} - 100}{100} \quad (8.16)$$

$$V = K \sqrt{\frac{\rho_L - \rho_V}{\rho_V}} \quad (8.17)$$

where,

Design pressure = 34.8 psi,

Density of liquid = 728.3 kg/m³,

Density of vapour = 0.189 kg/m³,

Vapour flow rate = $Q = 9.417 \text{ m}^3/\text{sec}$

$$K = 0.356$$

$$U = 11.045 \text{ ft/sec}$$

$$D = 1.88 \text{ m}$$

$$H = 8.57 \text{ m}$$

The vessel diameter is calculated based on the maximum allowable vapor velocity, V .

The thickness of flash (V-100) is calculated using correlation for the Cylindrical shell from Peter et. al.[9]

$$t = \frac{P \cdot r_i}{S - 0.6P} + C_c \quad (8.18)$$

Where, t = thickness, P = maximum allowable internal pressure, r_i = inside radius of the shell, C_c = allowance for corrosion, S = maximum allowable working stress

Costing

For cost estimation, formulae from Walas et. al have been used. The total cost is given by formula for Vertical vessels i.e., C . The following are the results for the vertical pressure column cost estimation as of Jan 2002.

For Vertical Vessels:

$$C = F_m C_b + C_a \quad (8.19)$$

$$C_a = 240 \cdot D^{0.7396} \cdot H^{0.7068} \quad (8.20)$$

$$C_b = 1.218 \cdot \exp(9.1 - 0.2889 \cdot \ln(W) + 0.04576 \cdot \ln(W)^2) \quad (8.21)$$

Where -

Outer diameter: $D_o = 1.88$ m

Thickness: $t = 9$ mm

$F_m = 2.1$

$C_b = 1858.78$

$C_a = 1747.47$

$$\text{Cost} = F_m C_b + C_a = \$12000$$

8.4 Distillation Column

For the design of our three Distillation Columns: T-100, T-101 and T-102 we have used formulae from Kister Henry Z[12], Peters et.al[9], Perry,R.H and Green[11].

The maximum allowable vapor velocity is found using the flooding velocity formula from Fair's correction of Souders-Brown equation. The $C_{sb,f}$ is a parameter found by an empirical correlation which decides the value of flooding velocity.

$$U_{flood} = C_{sb,f} \left(\frac{\sigma}{20} \right)^{0.2} \sqrt{\frac{\rho_L - \rho_V}{\rho_V}} \quad (8.22)$$

$$F_{lv} = \frac{W_L}{W_V} \sqrt{\frac{\rho_V}{\rho_L}} \quad (8.23)$$

$$\log(C_{sb,f}) = -1.0262 - 0.63513 \log(F_{lv}) - 0.20097 [\log(F_{lv})]^2 \quad (8.24)$$

where-

σ = Surface Tension in dyne/cm

F_{lv} = Flow parameter

W_L = Liquid Flow Rate in kg/h

W_V = Vapor Flow Rate in kg/h

$$\text{Dia} = \sqrt{\frac{4V}{\pi \cdot \rho_V \cdot U}} \quad (8.25)$$

where -

Dia = Diameter in m

V = Vapor flow rate in kg/s

U = Vapor velocity in m/s

Calculations For T-100:

- $W_L = 380919 \text{ kg/h}$, $W_V = 552192 \text{ kg/h}$
- $\rho_L = 547 \text{ kg/m}^3$, $\rho_V = 13 \text{ kg/m}^3$
- $F_{lv} = 0.22$, $C_{sb,f} = 0.20$
- $\sigma = 6.48 \text{ dyne/cm}$
- $U_{flood} = 1.03 \text{ m/s}$
- $V = \frac{380919}{3600} = 106 \text{ kg/s}$
- Diameter = 3.2 m
- Height = $\frac{\text{No. of Theoretical trays}}{\text{Efficiency}} \times \text{Tray spacing} = \frac{8}{0.7} \times 0.6 = 7 \text{ m}$

Column Thickness Calculation:

Since the distillation columns operate under a temperature of 300°C and a pressure of 300 kPa with non-corrosive components, Carbon Steel (SA-285) is chosen as the Material of Construction (MOC).

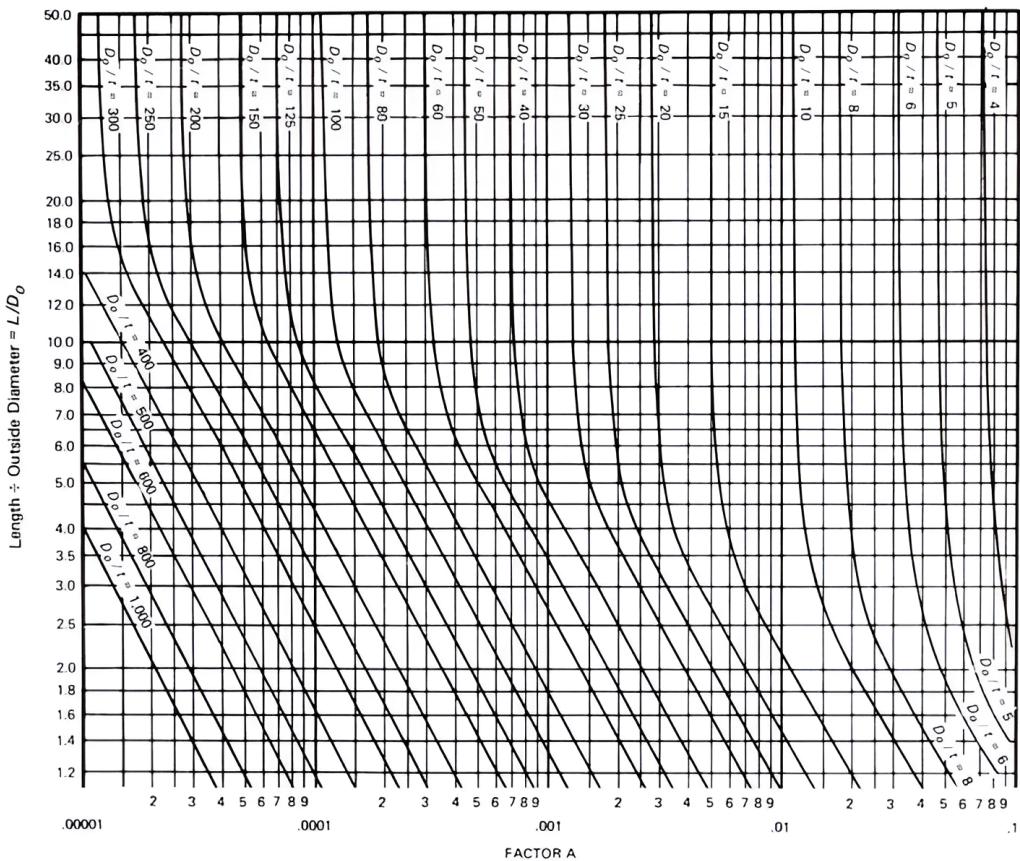


Figure 8.2: Geometric Chart of components under external Pressure

$$\text{Thickness} = \frac{Pr}{SE - 0.6P} + C \quad (8.26)$$

where:

P = Internal Pressure in kPa

r = Inside radius of the vessel in m

S = Yield point of material / Maximum allowable stress (for Carbon Steel SA-285 at 340°C, S = 94500 kPa)

E = Welding Efficiency (0.8)

C = Corrosion allowance (6 mm)

Using the above equation, the calculated thickness for T-100 is 13 mm.

The columns T-101 and T-102 operate under 20 kpa and 10 kpa respectively which come under near vacuum distillation. So we need to consider external Pressure and buckling strength to determine the thickness of the vessel. Charts from ASME BPVC code section- II part-D are used.

We have assumed a thickness t and determined the L/D and D/t ratios. Using these

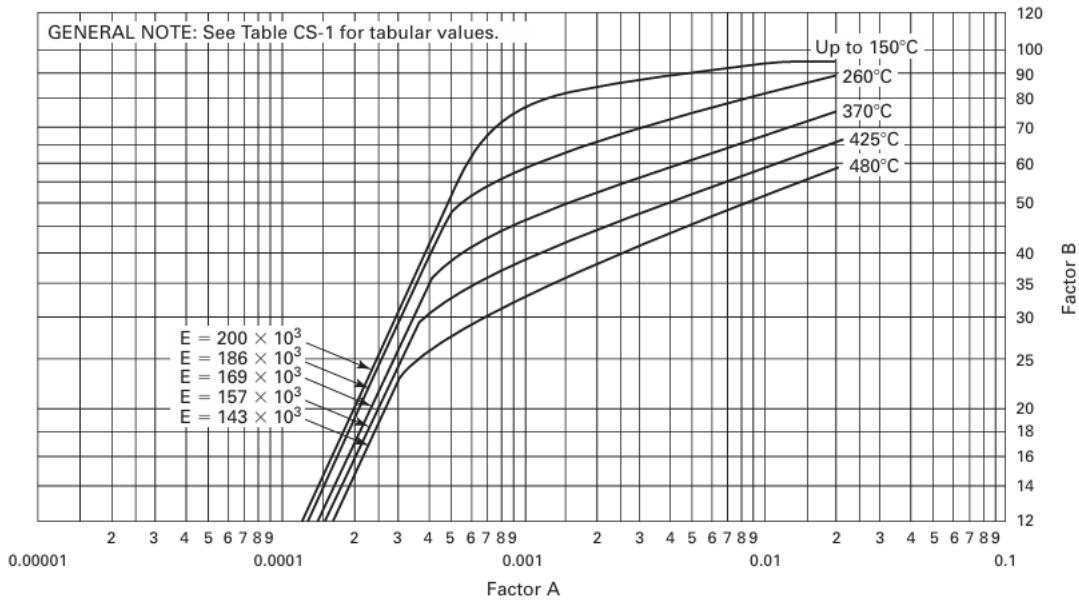


Figure 8.3: Chart for Determining Shell Thickness of Components Under External Pressure

ratios we have found geometric factor A from (figure 8.2). From Figure 8.3 we have found Factor B with the help of Factor and operating temperature. Using this factor B we have calculated maximum allowable external working pressure P.

$$P = \frac{4Bt}{D} \quad (8.27)$$

If the value of P is equal to or more than atmospheric pressure then our assumption is correct if not we choose new thickness and repeat the process again. By performing several iterations we have found out the value of the thickness to be 48 mm for T-101 and 32 mm for T-102.

Summary of Column Dimensions:

Table 8.5: Distillation Column Dimensions

Column	Diameter (m)	Height (m)	Thickness (mm)
T-100	3.2	7	13
T-101	4.8	10	48
T-102	2.5	7	32

Cost Estimation:

To estimate costs, we used nomograms from Peters et. al[9]. For finding the cost of the columns, we have to determine the weight of the vessels, including the shell, two heads, internals such as trays, manholes, reboiler, and condenser costs.

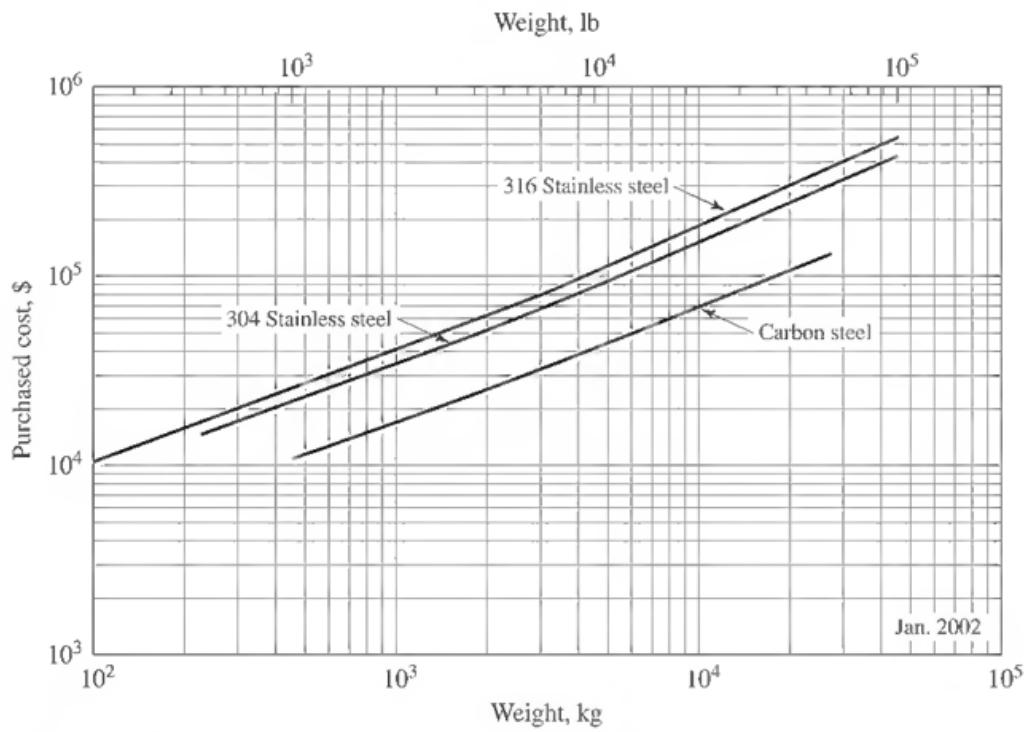


Figure 8.4: Cost vs weight of vessel

Calculation for T-100:

- Density of carbon steel = 7833 kg/m^3
- Weight of the vessel = weight of shell + weight of two heads
- $= \pi(D+t)th \cdot \text{density} + \frac{4}{3}\pi((D/2+t)^3 - (D/2)^3) \cdot \text{density}$
- $= 9900$
- Cost of the vessel weighing around 9900 kg is 70,000 USD (from figure 8.4)
- Since the liquid and vapor flow rate is very high, sieve trays are preferred
- Total Cost of 12 sieve trays for a 3.2 m diameter column is 12,600 USD (from figure 8.6)
- Total 2 manholes are considered, one for the top and one for the bottom
- Cost of 3 flanged manholes of 0.46 m internal diameter for a 13 mm thick vessel is 12,000 USD (from figure 8.5)
- Total Cost = 94,600 USD

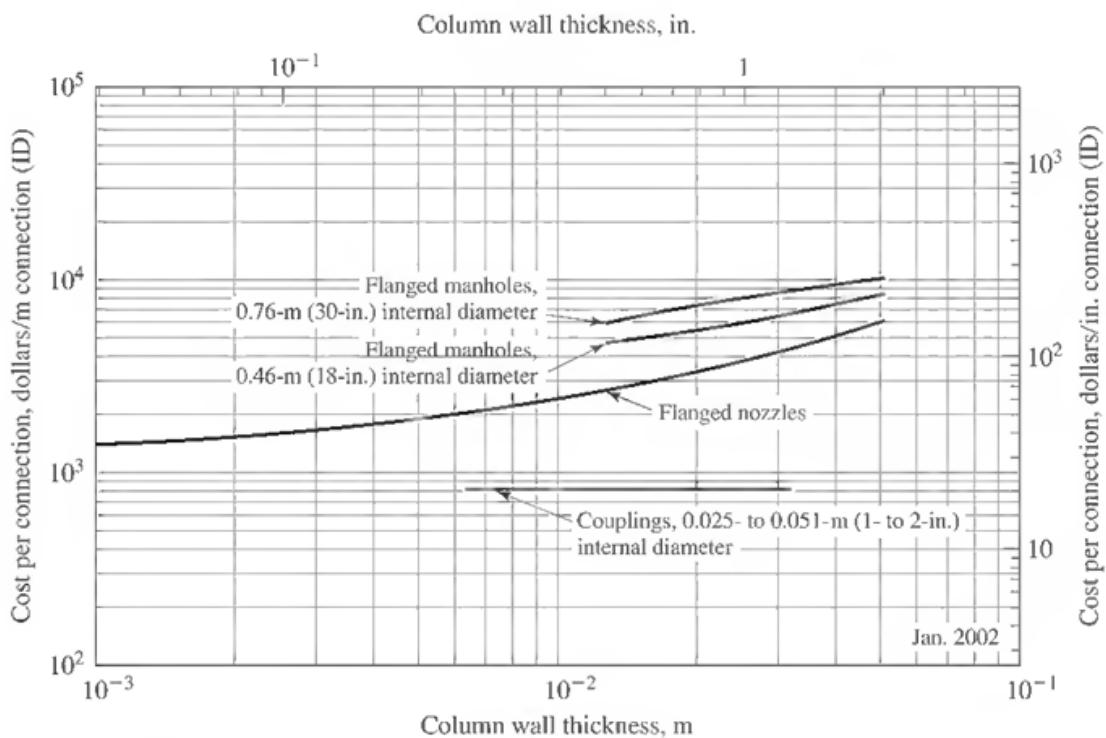


Figure 8.5: Cost of connections

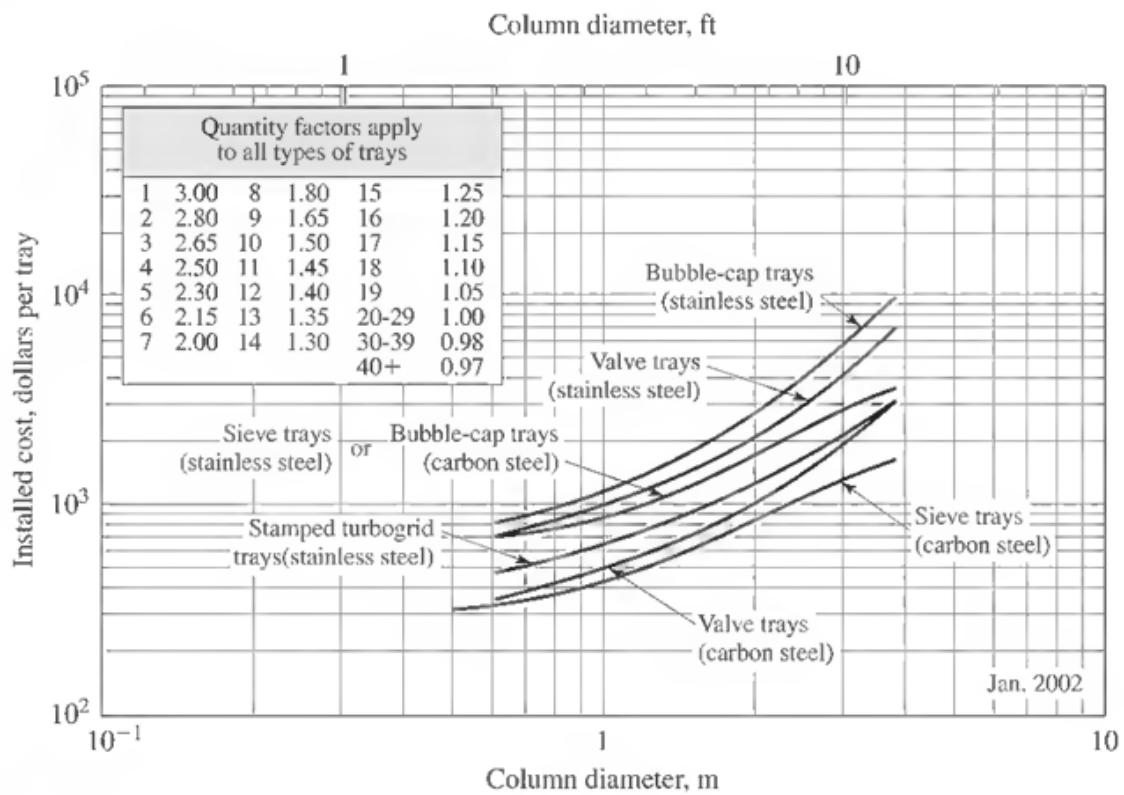


Figure 8.6: Cost of trays

Table 8.6: Cost Estimation for Distillation Columns

Specification	T-100	T-101	T-102	Total Cost (USD)
Cost of Vessel	70,000	250,000	100,000	420,000
Cost of Sieve Trays	12,600	13,200	9,000	34,800
Cost of Manholes	6,000	24,000	14,000	44,000
Total Cost	88,600	287,200	123,000	498,800

8.5 Heat Exchangers

Sample Calculation for E-100

Parameter	Value
Hot Fluid Inlet Temperature ($T_{h,in}$)	425.4 °C
Hot Fluid Outlet Temperature ($T_{h,out}$)	286.2 °C
Cold Fluid Inlet Temperature ($T_{c,in}$)	50 °C
Cold Fluid Outlet Temperature ($T_{c,out}$)	250 °C
Heat Duty (Q)	15,205,555 W

Temperature Effectiveness (P)

$$\begin{aligned}
 P &= \frac{T_{c,out} - T_{c,in}}{T_{h,in} - T_{c,in}} \\
 &= \frac{250 - 50}{425.4 - 50} \\
 &= \frac{200}{375.4} \\
 &= 0.5328
 \end{aligned}$$

Temperature Ratio (R)

$$\begin{aligned}
 R &= \frac{T_{h,in} - T_{h,out}}{T_{c,out} - T_{c,in}} \\
 &= \frac{425.4 - 286.2}{250 - 50} \\
 &= \frac{139.2}{200} \\
 &= 0.6960
 \end{aligned}$$

Correction Factor (F)

$$F = \frac{\sqrt{R^2 + 1}}{R - 1} \cdot \frac{\ln\left(\frac{1-P}{1-PR}\right)}{\ln\left(\frac{2-P(R+1-\sqrt{R^2+1})}{2-P(R+1+\sqrt{R^2+1})}\right)}$$

After substituting and calculating:

$$F \approx 0.8760$$

Log Mean Temperature Difference (LMTD)

$$\Delta_1 = T_{h,\text{in}} - T_{c,\text{out}} = 425.4 - 250 = 175.4$$

$$\Delta_2 = T_{h,\text{out}} - T_{c,\text{in}} = 286.2 - 50 = 236.2$$

$$\text{LMTD} = \frac{\Delta_1 - \Delta_2}{\ln(\Delta_1/\Delta_2)} = 204.2943 \text{ K}$$

Required Heat Transfer Area

$$\begin{aligned} A &= \frac{Q}{U \cdot F \cdot \text{LMTD}} \\ &= \frac{15,205,555}{1,336.2 \cdot 0.8760 \cdot 204.2943} \\ &= 64 \text{ m}^2 \end{aligned}$$

Cost Calculation

Heat exchangers cost estimation is done using correlations from Walas et al. based on the Chemical Engineering Plant Cost Index (1984). The total cost is given by:

$$C = f_c \cdot f_d \cdot f_m \cdot f_p \cdot C_b$$

Parameters

Parameter	Value
Surface Area	64 m ²
Exchanger Type	Fixed-head
Pressure	2.4 bar
Material	Stainless Steel 347

Base Cost Calculation

$$A_{ft^2} = 64 \times 10.7639 = 688.8 \text{ ft}^2$$

$$\ln(A_{ft^2}) = \ln(688.8) = 6.53$$

$$\begin{aligned} C_b &= \exp(8.821 - 0.30863 \times 6.53 + 0.0681 \times 41.5636) \\ &= 15,307.79 \end{aligned}$$

Type Factor Calculation

$$\begin{aligned}f_d &= \exp(-1.1156 + 0.0906 \times 6.4463) \\&= \exp(-0.5312) \\&= 0.5880\end{aligned}$$

Pressure Factor Calculation

$$\begin{aligned}f_p &= 0.7771 + 0.04981 \times 6.4463 \\&= 1.0987\end{aligned}$$

Material Factor Calculation

$$\begin{aligned}f_m &= 0.6116 + 0.22186 \times 6.4463 \\&= 2.0415\end{aligned}$$

Total Cost Estimation

$$\begin{aligned}C &= 1.21 \times 0.5880 \times 2.0415 \times 1.0987 \times 15,307.94 \\&= 24,424\end{aligned}$$

Cost Breakdown Analysis

Component	Value
Base Cost	\$15,307.79
Type Factor	0.5880
Material Factor	2.0415
Pressure Factor	1.0987
Final Multiplier	1.21
Estimated Total Cost in 2002	\$24,424
Estimated Total Cost in 2024 in India	30.72 lakh

Similar calculations were carried out for other heat exchangers and their results are tabulated below. (Table 8.7, 8.8, 8.9)

Heat Exchangers	E-100	E-101	E-102	E-103
Shell Side				
Fluid	Paraffin	Paraffin	Chilled Water	Paraffin+Olefin
T_{Inlet} (°C)	50	200	7	50
T_{Outlet} (°C)	250	450	25	75
Pressure (Bar)	2.4	2.4	2.4	2.4
MOC	SS 347	SS 347	SS 316	SS 304
Tube Side				
Fluid	Paraffin+Olefin	Thermal Fluid	Paraffin+Olefin	LP Steam
T_{Inlet} (°C)	425	750	217	135
T_{Outlet} (°C)	286	500	50	110
Pressure (Bar)	2.4	2.4	2.4	2.4
MOC	SS 347	SS 347	SS 316	SS 304
Performance and Costing				
Heat Load (kW)	15205	26558	23980	1618
Overall Heat Transfer Coefficient (W/(m²K))	1336	492	943	634
ΔT_{LMTD} (°C)	204	300	99	75
F	0.87	1	0.94	1
Area Required (m²)	64	180	272	34
Cost for 2002 (\$)	24,424	67455	115236	15033

Table 8.7: Shell and Tube Heat Exchanger Parameters and Costing

Heat Exchangers	E-104	E-105	E-106	E-107
Shell Side				
Fluid	Benzene	Chilled Water	LAB+Paraffin	Cooling Water
T_{Inlet} (°C)	75	7	266	35
T_{Outlet} (°C)	90	25	273	50
Pressure (Bar)	3	3	2	3
MOC	SS 304	CS 304	CS 316	SS 304
Tube Side				
Fluid	LP Steam	Paraffin	Thermal Fluid	Benzene
T_{Inlet} (°C)	200	95	350	104
T_{Outlet} (°C)	140	50	300	74
Pressure (Bar)	3	3	2	3
MOC	SS 304	CS 304	CS 316	SS 304
Performance and Costing				
Heat Load (kW)	605	2675	1264.11	4143.07
Overall Heat Transfer Coefficient (W/(m²K))	450	1068	480	1530
ΔT_{LMTD} (°C)	85	55	52	72
F	1	0.95	0.97	0.98
Area Required (m²)	16	47	131	198
Cost for 2002 (\$)	9050	19233	57915	65450

Table 8.8: Shell and Tube Heat Exchanger Parameters and Costing

Heat Exchangers	E-108	E-109	E-110	E-111
Shell Side				
Fluid	LAB+HAB	Cooling Water	HAB	Cooling Water
T_{Inlet} (°C)	242	35	233	35
T_{Outlet} (°C)	253	50	240	75
Pressure (Bar)	0.2	0.02	0.1	0.02
MOC	SS 304	SS 304	SS 304	SS 304
Tube Side				
Fluid	Thermal Fluid	Paraffin	Thermal Fluid	LAB
T_{Inlet} (°C)	350	97	350	184
T_{Outlet} (°C)	260	95	300	182
Pressure (Bar)	0.2	0.02	0.1	0.02
MOC	SS 304	SS 304	SS 304	SS 304
Performance and Costing				
Heat Load (kW)	9076	21938	2399	3300
Overall Heat Transfer Coefficient (W/(m²K))	1420	1256	1268	1308
ΔT_{LMTD} (°C)	46	79	86	127
F	0.90	0.99	0.99	0.99
Area Required (m²)	150	220	22	20
Cost for 2002 (\$)	50654	72059	110393	10375

Table 8.9: Shell and Tube Heat Exchanger Parameters and Costing

Chapter 9

Plant Economics

This chapter focuses on an overview of the plant economics, by estimating the capital investments, production costs and the payback period for the Linear Alkyl Benzene production plant.

The following data are used for the cost estimation:

- India location factor w.r.t US = 0.7
- Dollar to INR = 85
- Cost Index - Chemical Engineering Plant Cost Index
- All equipment are mapped to the average 2024 Cost Index - 800

9.1 Major equipment Costing

The Linear Alkylbenzene plant has many major equipment which includes storage tanks, pumps, heat exchangers, reactors, flash and distillation columns. Nomograms and correlations from Peters et. al.[9] and Walas et. al.[10] have helped us arrive at the total purchased cost of these equipment. The following table(9.1) presents the total purchased and delivered cost of all equipment.

Table 9.1: Total equipment costing

Equipment	Total equipment cost (\$ in 2002)
Reactor	0.5 Million
Storage tanks	2.21 Million
Pumps	0.17 Million
Heat exchangers	0.52 Million
Distillation Columns	0.5 Million
Flash tower	0.007 Million
Total Equipment Cost (FOB)	3.907 Million
Total Equipment Cost (Delivered)	4.298 Million

9.2 Capital Investment Estimation

The equipments cost of major equipments in earlier chapter are used to calculate the total capital investment in the plant. The plant is considered to be a Fluid-Fluid Processing plant. Working capital is taken to be as 15% of the total capital investment. The total capital investment is determined using the method of percentage of delivered equipment cost. India factor is considered to be 0.7.

The results of the analysis are as given in the table(9.2) :

Table 9.2: Capital Investment Estimation

Direct costs	Percentage	Normalized Cost	Cost (million \$ as in 2002)
Purchase Equipment Delivered	100	0.20	4.298
Purchased Equipment Installation	47	0.09	2.02
Instrumentation and controls	36	0.07	1.54
Piping	68	0.13	3.02
Electrical Systems	11	0.02	0.52
Buildings	18	0.04	0.77
Yard Improvements	10	0.02	0.43
Service Facilities	70	0.14	3.00
Land	5	0.01	0.22
Total direct plant cost	365	0.72	15.69
Indirect cost			
Engineering and Supervision	33	0.06	1.42
Construction Expenses	41	0.08	1.76
Legal Expenses	4	0.01	0.17
Contractor's Fee	22	0.04	0.94
Contingency	44	0.09	1.89
Total indirect plant cost	144	0.28	6.18
Fixed Capital Investment	509	1	21.87
Working capital (15 % of TCI)	90	0.18	3.86
TCI (according to USA, in 2002)			25.74
India factor			0.7
TCI (according to India, in 2002)			18.02
TCI (according to India, in 2024)			37.35

India factor of 0.7 has been used. The cost has been scaled to 2019 value using CEPCI cost index. $CEPCI_{2002} = 368$, $CEPCI_{2024} = 800$

Using an exchange rate of 85 INR = \$1, we estimate the final value:

Total Capital investment = 323.83 Crore INR (in 2024)

9.3 Raw Material Cost

The total product cost can be estimated after estimating the cost of raw materials(Table(9.3)). The raw material for this process are benzene and paraffin.

Table 9.3: Raw material cost

	Amount (tons/yr)	Cost (\$/ton)	Cost \$/yr	Cost INR/yr
Benzene	44992	640	28.956 Million	247.45 Crore
Paraffin	100840	880	88.411 Million	756.30 Crore

Hence, total raw material cost = 1003.75 Crore INR/year

9.4 Revenue Calculation

The main product which is Linear Alkylbenzene is sold at 190 INR, as shown in table 9.4.

Table 9.4: Revenue calculation

	Amount (tons/yr)	Cost	Price \$/yr
Linear Alkylbenzene	139736	2162 \$/ton	31.03 million

Hence, total revenue = \$31.03 Million = 2654.98 Crore INR/year

9.5 Total Product Cost

Total Product cost is calculated using normalised percentage method from Peters et. al as shown in table 9.5. Since the plant is set up in India, India factor of 0.7 is applied to Operating Labour, Supervising Labour and Admin costs.

Table 9.5: Total product cost estimation

Category	Factor	Normalized	Cost \$/yr
Raw material	50	0.39	115.8 Million
Operating Labour	10	0.08	16.2 Million
Supervising Labour	2	0.02	3.2 Million
Utilities	15	0.12	34.73 Million
Repairs and Maintenance	7	16.2	Million
Operating supplies	1.05	0.01	2.43 Million
Laboratory charges	1	0.01	2.31 Million
Patents	3	0.02	6.94 Million
Fixed charges	13	0.10	30.10 Million
Plant overhead	9.5	0.07	21.99 Million
Admin costs	1.5	0.01	2.43 Million
Distribution and marketing	11	0.09	25.47 Million
R&D cost	5	0.04	11.57 Million
Total product cost	129.05	1.00	298.81 Million

Hence, total product cost = \$298.81 Million = 2590.7 Crore INR/year

9.6 Payback Period

The following assumptions have been made while calculating the payback period:

1. 90% of FCI excluding the land costs is considered to be depreciable over a period of 10 years.
2. Average depreciation is calculated using a linear depreciation model.
3. Bank interest rate of 6% over the total capital used.
4. Capacity is 70% 1st year, 80% 2nd year, and 90% from 3rd year onwards

The following values are in Crore INR, at 100% production:

- Total depreciable FCI = INR 245.23 Crores
- Total depreciable per yr = INR 24.52 Crore
- Tax rate = 25%
- Taxation rate (including surcharge and cess) = 27.5%
- Gross Profit before depreciation = Revenue - Total product cost = INR 200.248 Crores

- Net Profit = (Gross profit - depreciation) \times (1 - tax rate) = INR 64.3 Crores

The following table(9.6) shows the cash flow from the plant production.

Table 9.6: Payback period calculation

Year	Capacity (%)	Invest-ment	Cost	Revenue	Gross profit	Depre-ciation	Net Profit	Cumulative position
0		-323.83						-323.83
1	70		-1813.48	1858.48	45	24.52	14.84	-284.46
2	80		-2072.55	2123.98	51.43	24.52	19.5	-240.43
3	90		-2331.62	2389.48	57.96	24.52	24.16	-191.74
4	90		-2331.62	2389.48	57.96	24.52	24.16	-143.05
5	90		-2331.62	2389.48	57.96	24.52	24.16	-94.35
6	90		-2331.62	2389.48	57.96	24.52	24.16	-45.66
7	90		-2331.62	2389.48	57.96	24.52	24.16	-3.02
8	90		-2331.62	2389.48	57.96	24.52	24.16	-51.72
9	90		-2331.62	2389.48	57.96	24.52	24.16	-100.41
10	90		-2331.62	2389.48	57.96	24.52	24.16	-149.10

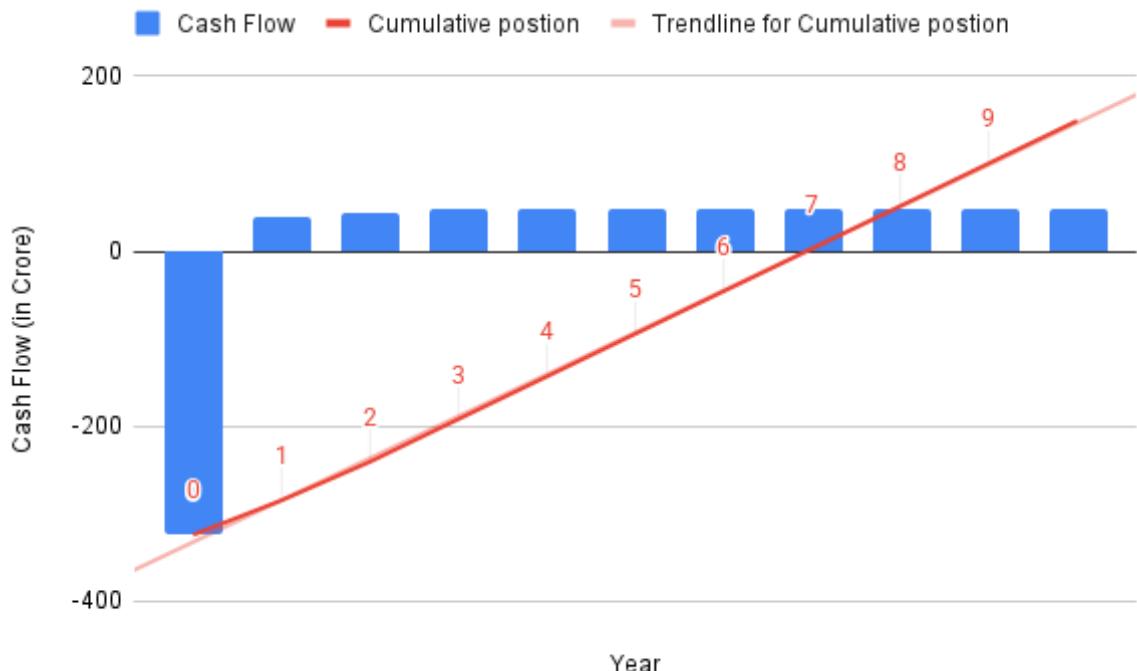


Figure 9.1: Estimated cash flow from plant operation

Hence, Payback period ~ 7 years as shown in figure 9.1

Chapter 10

Detailed Design of Heat Exchangers

10.1 Introduction

Shell and tube heat exchangers are widely used in industrial applications due to their versatility and reliability. This report documents the detailed design procedure for a shell and tube heat exchanger based on specific process requirements. The design process follows standard heat exchanger design methodologies, ensuring thermal performance while considering practical engineering constraints.

10.2 Process Parameters

The design of the heat exchanger is based on the following process parameters:

10.2.1 Temperature Requirements

For the hot fluid (shell side):

$$T_{h,in} = 425.4^\circ\text{C} \quad (\text{inlet temperature})$$

$$T_{h,out} = 286.2^\circ\text{C} \quad (\text{outlet temperature})$$

For the cold fluid (tube side):

$$T_{c,in} = 50^\circ\text{C} \quad (\text{inlet temperature})$$

$$T_{c,out} = 250^\circ\text{C} \quad (\text{outlet temperature})$$

10.2.2 Heat Duty

The required heat transfer rate for the exchanger:

$$Q = 15\,205\,555 \text{ W} \quad (\text{or approximately } 15.2 \text{ MW})$$

These parameters establish the thermal requirements that our heat exchanger design must satisfy. The significant temperature difference between the hot and cold fluids indicates the potential for efficient heat transfer, while the substantial heat duty

suggests that careful attention must be paid to the heat transfer area and coefficient calculations.

10.3 Log Mean Temperature Difference (LMTD) Calculation

The Log Mean Temperature Difference (LMTD) is a fundamental parameter in heat exchanger design that represents the effective driving force for heat transfer. For a counter-current flow arrangement, the LMTD is calculated as follows:

10.3.1 Temperature Differences

First, we calculate the temperature differences at both ends of the heat exchanger:

$$\begin{aligned}\Delta T_1 &= T_{h,in} - T_{c,out} \\ &= 425.4^\circ\text{C} - 250^\circ\text{C} \\ &= 175.4\text{ K}\end{aligned}$$

$$\begin{aligned}\Delta T_2 &= T_{h,out} - T_{c,in} \\ &= 286.2^\circ\text{C} - 50^\circ\text{C} \\ &= 236.2\text{ K}\end{aligned}$$

10.3.2 LMTD Formula

The LMTD is then calculated using the logarithmic mean formula:

$$\begin{aligned}\text{LMTD} &= \frac{\Delta T_1 - \Delta T_2}{\ln(\Delta T_1 / \Delta T_2)} \\ &= \frac{175.4 - 236.2}{\ln(175.4 / 236.2)} \\ &= 204.29\text{ K}\end{aligned}$$

10.4 Correction Factor Calculation

For a shell and tube heat exchanger with multiple tube passes, the LMTD must be adjusted using a correction factor F . This correction accounts for the deviation from ideal counter-current flow due to the multiple passes arrangement.

10.4.1 Thermal Effectiveness Parameters

First, we calculate the thermal effectiveness parameters P and R :

$$\begin{aligned} P &= \frac{T_{c,out} - T_{c,in}}{T_{h,in} - T_{c,in}} \\ &= \frac{250 - 50}{425.4 - 50} \\ &= 0.5328 \end{aligned}$$

$$\begin{aligned} R &= \frac{T_{h,in} - T_{h,out}}{T_{c,out} - T_{c,in}} \\ &= \frac{425.4 - 286.2}{250 - 50} \\ &= 0.6960 \end{aligned}$$

10.4.2 Correction Factor Formula

For a 1-2 shell and tube heat exchanger (one shell pass and two tube passes), the correction factor F is calculated using:

$$F = \frac{\sqrt{R^2 + 1}}{R - 1} \cdot \frac{\ln\left(\frac{1-P}{1-PR}\right)}{\ln\left(\frac{2-P(R+1-\sqrt{R^2+1})}{2-P(R+1+\sqrt{R^2+1})}\right)}$$

Substituting our values:

$$\begin{aligned} F &= \frac{\sqrt{0.6960^2 + 1}}{0.6960 - 1} \cdot \frac{\ln\left(\frac{1-0.5328}{1-0.5328 \times 0.6960}\right)}{\ln\left(\frac{2-0.5328(0.6960+1-\sqrt{0.6960^2+1})}{2-0.5328(0.6960+1+\sqrt{0.6960^2+1})}\right)} \\ &= \frac{\sqrt{0.4844 + 1}}{-0.304} \cdot \frac{\ln\left(\frac{0.4672}{0.6292}\right)}{\ln\left(\frac{2-0.5328(1.6960-1.2140)}{2-0.5328(1.6960+1.2140)}\right)} \\ &= 0.8760 \end{aligned}$$

The correction factor of 0.8760 indicates that our heat exchanger's effective temperature difference is approximately 87.6% of the ideal counter-current LMTD. This reduction is due to the flow arrangement in the 1-2 shell and tube design. A correction factor greater than 0.8 is generally considered acceptable for practical heat exchanger designs.

10.5 Initial Area Estimation

To begin the iterative design process, we make an initial estimation of the required heat transfer area based on an assumed overall heat transfer coefficient.

10.5.1 Initial Heat Transfer Coefficient Assumption

We start with an initial guess for the overall heat transfer coefficient:

$$U_{guess} = 5000 \text{ W/m}^2 \cdot \text{K}$$

This is a reasonable starting point based on typical values for shell and tube heat exchangers with similar fluids.

10.5.2 Required Heat Transfer Area

The required heat transfer area is calculated using:

$$\begin{aligned} A &= \frac{Q}{U \times F \times \text{LMTD}} \\ &= \frac{15,205,555}{5000 \times 0.8760 \times 204.29} \\ &= 17.0 \text{ m}^2 \end{aligned}$$

10.5.3 Initial Tube Count Estimation

Based on the preliminary area estimation, we can calculate the initial number of tubes required:

$$N_{\text{tubes}} = \frac{A}{\pi \times d_o \times L}$$

Assuming standard tube dimensions(taken from TEMA standard) :

$$d_o = 0.025 \text{ m} \quad (\text{outer diameter})$$

$$L = 6.10 \text{ m} \quad (\text{tube length})$$

Substituting these values:

$$\begin{aligned} N_{\text{tubes}} &= \frac{17.0}{\pi \times 0.025 \times 6.10} \\ &= \frac{17.0}{0.4786} \\ &\approx 35.5 \end{aligned}$$

Rounding up to the next integer:

$$N_{\text{tubes}} \approx 36 \text{ tubes}$$

This initial estimation provides a starting point for our detailed heat exchanger design. The actual number of tubes will be refined through subsequent iterations as we calculate more accurate heat transfer coefficients.

10.6 Shell & Tube Parameters

10.6.1 Tube Dimensions

The tube dimensions are selected based on standard commercial sizes and practical considerations:

$$d_o = 0.025 \text{ m} \quad (\text{outer diameter})$$

$$d_i = 0.021 \text{ m} \quad (\text{inner diameter})$$

$$L = 6.10 \text{ m} \quad (\text{tube length})$$

The tube thickness is therefore:

$$\begin{aligned} t &= \frac{d_o - d_i}{2} \\ &= \frac{0.025 - 0.021}{2} \\ &= 0.002 \text{ m} \quad (2 \text{ mm}) \end{aligned}$$

10.6.2 Bundle Diameter Calculation

The tube bundle diameter is calculated using empirical correlations that relate the number of tubes to the bundle diameter:

$$D_b = d_o \times \left(\frac{N_{\text{tubes}}}{k_1} \right)^{1/n_1}$$

For a shell and tube heat exchanger with 1 shell pass and 2 tube passes, the constants are taken from Table 10.1

$$k_1 = 0.249$$

$$n_1 = 2.207$$

Table 10.1: Coefficients for Different Pitch Arrangements

Triangular pitch, $p_T = 1.25d_o$					
No. passes	1	2	4	6	8
K_1	0.319	0.249	0.175	0.0743	0.0365
n_1	2.142	2.207	2.285	2.499	2.675
Square pitch, $p_T = 1.25d_o$					
No. passes	1	2	4	6	8
K_1	0.215	0.156	0.158	0.0402	0.0331
n_1	2.207	2.291	2.263	2.617	2.643

Substituting our values:

$$D_b = 0.025 \times \left(\frac{36}{0.249} \right)^{1/2.207}$$

$$\approx 0.23 \text{ m}$$

10.6.3 Shell Diameter Calculation

The shell diameter is typically larger than the bundle diameter to allow for proper flow distribution and mechanical clearance:

$$D_s = D_b + \Delta$$

Where Δ is the clearance between the bundle and shell. For this design:

$$\Delta = 0.01 \text{ m}$$

$$D_s = 0.23 + 0.01$$

$$= 0.24 \text{ m}$$

10.7 Shell-Side Heat Transfer

The shell-side heat transfer coefficient is a critical parameter in determining the overall heat transfer performance of the exchanger. In this section, we calculate the various factors affecting shell-side heat transfer.

Used for the to find out the clearance between the bundle and shell

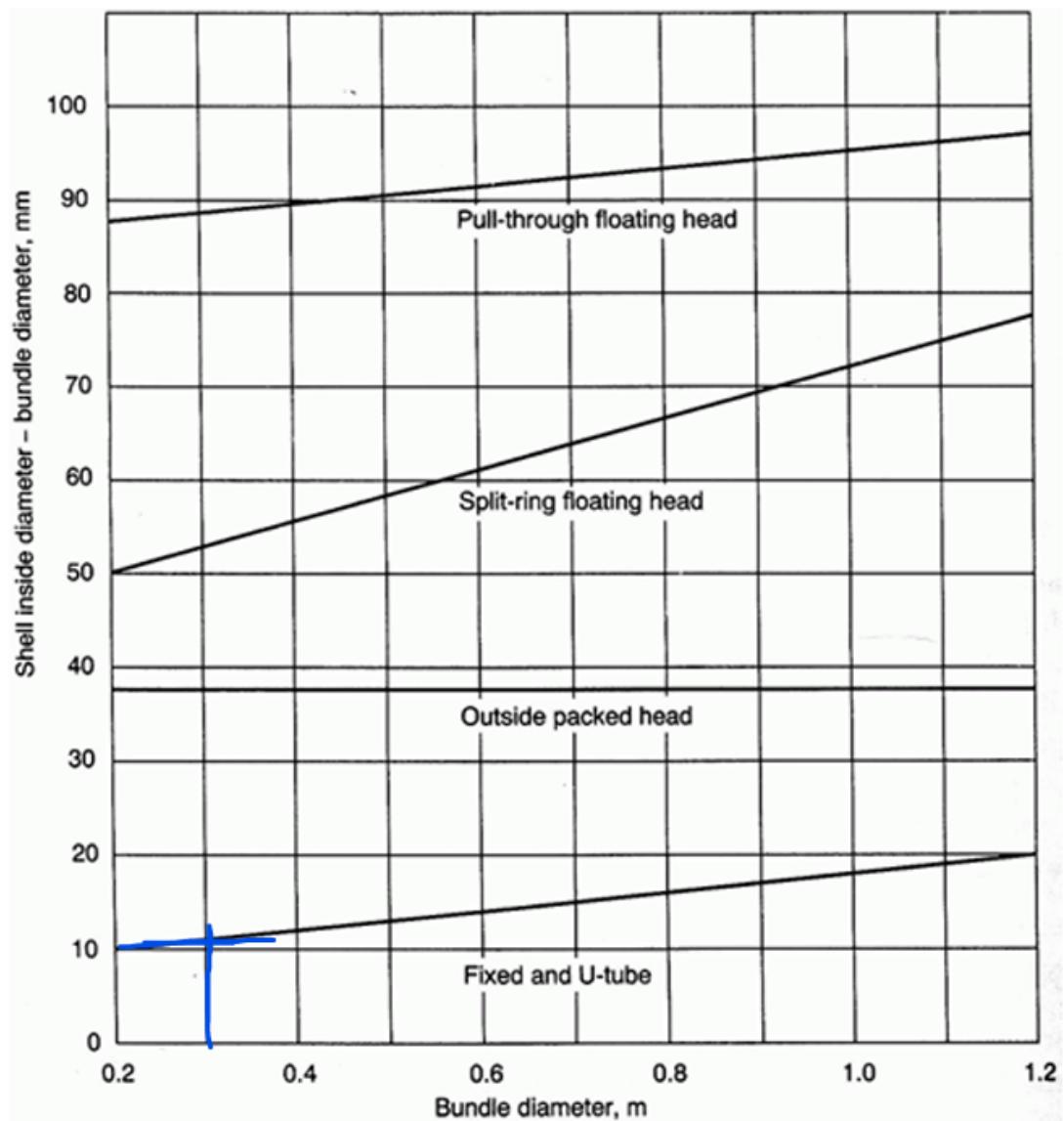


Figure 10.1: Find out the clearance between the bundle and shell

10.7.1 Tube Layout and Pitch

We select a triangular tube layout, which generally provides higher heat transfer rates compared to square layouts:

$$\text{Pitch type} = \text{triangular}$$

The tube pitch (center-to-center distance between adjacent tubes) is calculated as:

$$\begin{aligned} p_t &= 1.25 \times d_o \\ &= 1.25 \times 0.025 \\ &= 0.03125 \text{ m} \end{aligned}$$

10.7.2 Equivalent Diameter Calculation

For heat transfer calculations in the shell side with triangular pitch, the equivalent (hydraulic) diameter is calculated using:

$$\begin{aligned} d_e &= \frac{1.10}{d_o} \times (p_t^2 - 0.917 \times d_o^2) \\ &= \frac{1.10}{0.025} \times (0.03125^2 - 0.917 \times 0.025^2) \\ &\approx 0.017 \text{ m} \end{aligned}$$

10.7.3 Baffle Design

Baffles are essential components in shell and tube heat exchangers that direct the shell-side fluid flow across the tube bundle, enhancing heat transfer.

Minimum Baffle Spacing

The minimum baffle spacing is typically set as a fraction of the shell diameter:

$$\begin{aligned} b_{\min} &= 0.5 \times D_s \\ &= 0.5 \times 0.24 \\ &= 0.12 \text{ m} \end{aligned}$$

Number of Baffle Chambers

The number of baffle chambers along the tube length is calculated as:

$$\begin{aligned}N_c &= \frac{L}{b_{\min}} \\&= \frac{6.10}{0.12} \\N_c &\approx 50 \text{ chambers}\end{aligned}$$

Actual Baffle Spacing

Based on the determined number of chambers, we recalculate the actual baffle spacing:

$$\begin{aligned}b &= \frac{L}{N_c} \\&= \frac{6.10}{50} \\&\approx 0.122 \text{ m}\end{aligned}$$

10.7.4 Shell-Side Flow Area

The cross-sectional area available for shell-side fluid flow is calculated as:

$$\begin{aligned}A_s &= \frac{(p_t - d_o) \times D_s \times b}{p_t} \\&= \frac{(0.03125 - 0.025) \times 0.24 \times 0.122}{0.03125} \\&\approx 0.006153 \text{ m}^2\end{aligned}$$

10.7.5 Shell-Side Mass Velocity

The mass velocity in the shell side is calculated using the mass flow rate and the cross-sectional area:

$$\begin{aligned}G_s &= \frac{\dot{m}_s}{A_s} \\&= \frac{1.108 \times 10^5 / 3600}{0.006153} \\&= \frac{30.78}{0.006153} \\&\approx 5001.6 \text{ kg/m}^2 \cdot \text{s}\end{aligned}$$

10.7.6 Shell-Side Reynolds Number

The Reynolds number characterizes the flow regime and is essential for heat transfer coefficient calculations:

$$\begin{aligned}\text{Re} &= \frac{G_s \times d_e}{\mu} \\ &= \frac{5001.6 \times 0.017}{3.217 \times 10^{-5}} \\ &\approx 2.75 \times 10^6\end{aligned}$$

This high Reynolds number indicates highly turbulent flow in the shell side, which is beneficial for heat transfer.

10.7.7 Shell-Side Prandtl Number

The Prandtl number relates the momentum diffusivity to thermal diffusivity:

$$\begin{aligned}\text{Pr} &= \frac{c_p \times \mu}{k} \\ &= \frac{(3.742 \times 1000) \times (3.217 \times 10^{-5})}{0.1911} \\ &\approx 0.63\end{aligned}$$

10.7.8 Shell-Side Nusselt Number

For turbulent flow in the shell side, the Nusselt number is calculated using empirical correlations:

$$\begin{aligned}\text{Nu} &= j_h \times \text{Re} \times \text{Pr}^{0.33} \\ &= 0.0013 \times (2.75 \times 10^6) \times (0.63)^{0.33} \\ &\approx 3080\end{aligned}$$

10.7.9 Shell-Side Heat Transfer Coefficient

The shell-side heat transfer coefficient is calculated from the Nusselt number:

$$\begin{aligned}h_o &= \frac{\text{Nu} \times k}{d_e} \\ &= \frac{3080 \times 0.1911}{0.017} \\ &\approx 33161 \text{ W/m}^2 \cdot \text{K}\end{aligned}$$

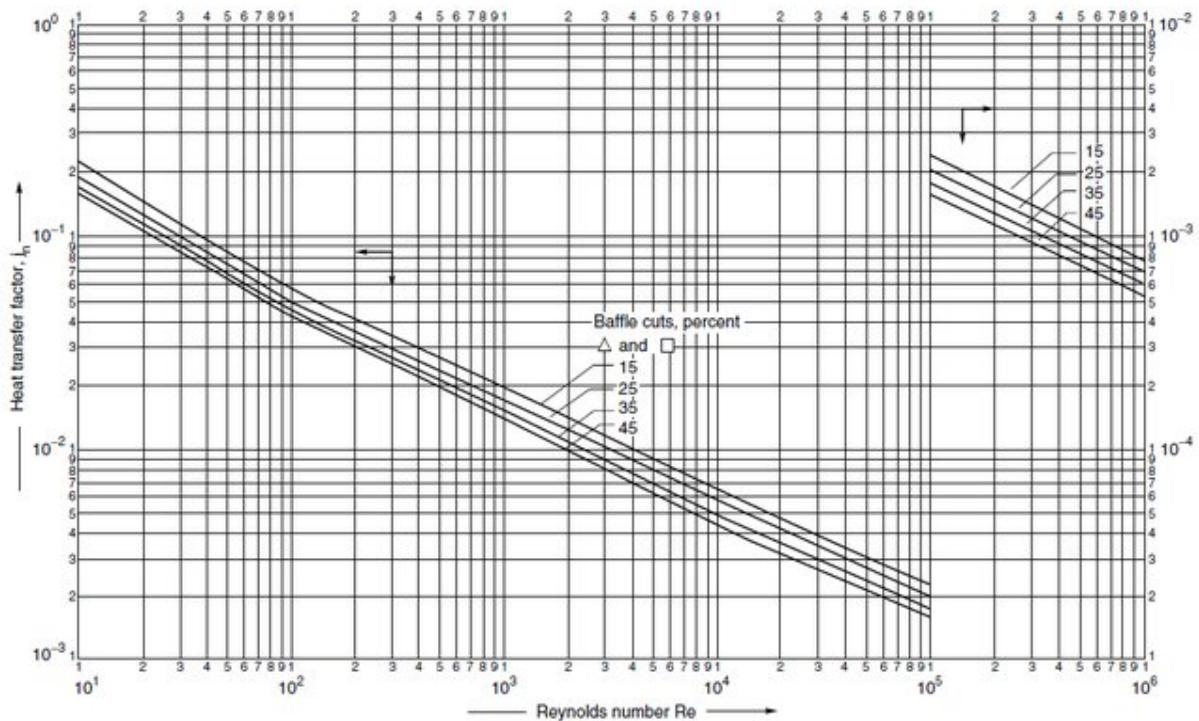


Figure 10.2: Shell side heat transfer factor

This high heat transfer coefficient reflects the turbulent flow conditions and efficient heat transfer in the shell side of our exchanger.

10.8 Tube-Side Heat Transfer

The tube-side heat transfer coefficient is another critical parameter in determining the overall heat transfer performance of the exchanger. In this section, we calculate the various factors affecting tube-side heat transfer.

10.8.1 Tube-Side Reynolds Number

The Reynolds number for the tube-side flow is calculated as:

$$\begin{aligned}
 \text{Re} &= \frac{4\dot{m}_t}{\pi\mu d_i} \\
 &= \frac{4 \times 29.14}{\pi \times (0.9154 \times 10^{-3}) \times 0.021} \\
 &= \frac{116.56}{\pi \times (0.9154 \times 10^{-3}) \times 0.021} \\
 &= \frac{116.56}{0.0000603} \\
 &\approx 1.93 \times 10^6
 \end{aligned}$$

This high Reynolds number indicates highly turbulent flow in the tubes, which is advantageous for heat transfer.

10.8.2 Tube-Side Prandtl Number

The Prandtl number for the tube-side fluid is calculated as:

$$\begin{aligned}\text{Pr} &= \frac{c_p \times \mu}{k} \\ &= \frac{1.763 \times 1000 \times 0.9154 \times 10^{-3}}{0.1306} \\ &= \frac{1.614}{0.1306} \\ &\approx 12.35\end{aligned}$$

10.8.3 Tube-Side Nusselt Number

For turbulent flow in circular tubes ($\text{Re} > 4000$), the Nusselt number is calculated using the Dittus-Boelter correlation with a correction factor for temperature-dependent properties:

$$\begin{aligned}\text{Nu} &= j_h \times \text{Re}^{0.8} \times \text{Pr}^{0.4} \times \left(1 + \frac{d_o}{L}\right)^{0.7} \\ &= 0.023 \times (1.93 \times 10^6)^{0.8} \times (12.35)^{0.4} \times \left(1 + \frac{25}{610}\right)^{0.7} \\ &\approx 6904\end{aligned}$$

10.8.4 Tube-Side Heat Transfer Coefficient

The tube-side heat transfer coefficient is calculated from the Nusselt number:

$$\begin{aligned}h_i &= \frac{\text{Nu} \times k}{d_i} \\ &= \frac{6904 \times 0.1306}{0.021} \\ &\approx 42941 \text{ W/m}^2 \cdot \text{K}\end{aligned}$$

This high heat transfer coefficient indicates efficient heat transfer within the tubes of our exchanger.

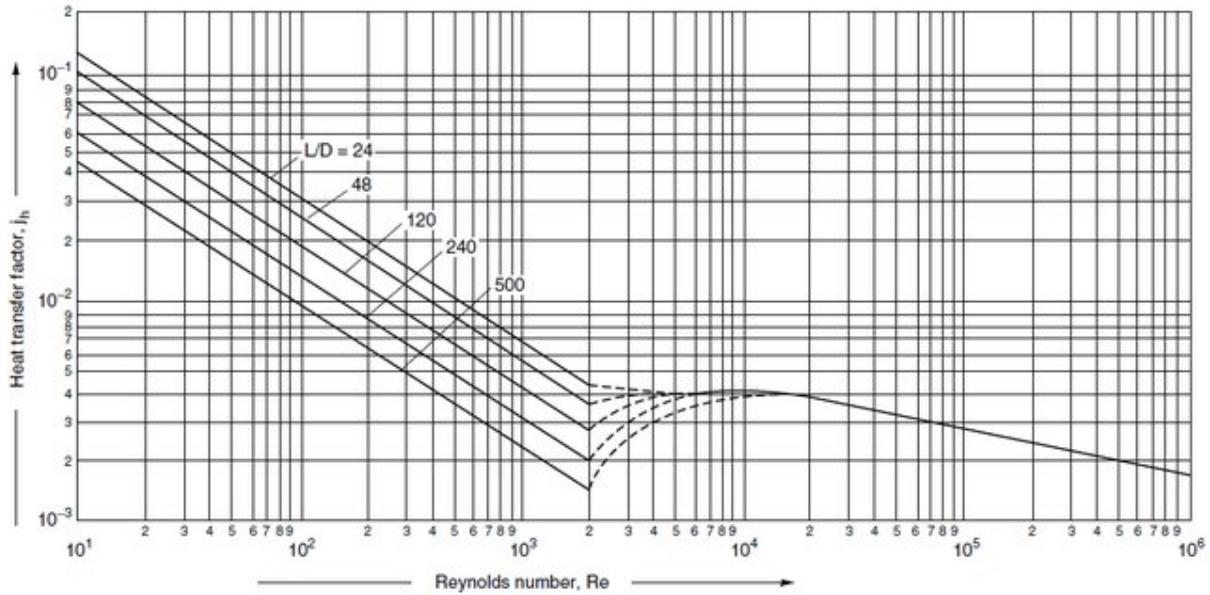


Figure 10.3: Tube side heat transfer factor

10.9 Overall Heat Transfer Coefficient

The overall heat transfer coefficient incorporates all thermal resistances in the heat exchanger, including convection on both sides, conduction through the tube wall, and fouling resistances.

10.9.1 Thermal Resistance Components

The overall heat transfer coefficient is calculated as the reciprocal of the total thermal resistance:

$$U = \frac{1}{R_{total}} = \frac{1}{\frac{1}{h_o} + \frac{1}{h_{od}} + \frac{d_o \times \ln(d_o/d_i)}{2 \times k_w} + \frac{d_o}{d_i} \left(\frac{1}{h_{id}} + \frac{1}{h_i} \right)}$$

Where:

$$h_o = 33161 \text{ W/m}^2 \cdot \text{K} \quad (\text{shell-side convection coefficient})$$

$$h_{od} = 5000 \text{ W/m}^2 \cdot \text{K} \quad (\text{shell-side fouling resistance})$$

$$k_w = 36 \text{ W/m} \cdot \text{K} \quad (\text{tube material thermal conductivity})$$

$$h_{id} = 5000 \text{ W/m}^2 \cdot \text{K} \quad (\text{tube-side fouling resistance})$$

$$h_i = 42941 \text{ W/m}^2 \cdot \text{K} \quad (\text{tube-side convection coefficient})$$

Substituting the values into the equation:

$$U = \frac{1}{\frac{1}{33161} + \frac{1}{5000} + \frac{0.025 \times \ln(0.025/0.021)}{2 \times 36} + \frac{0.025}{0.021} \left(\frac{1}{5000} + \frac{1}{42941} \right)} \\ \approx 1450 \text{ W/m}^2 \cdot \text{K}$$

Table 10.2: Value of shell side and tube side fouling resistance

Fluid	Coefficient ($\text{W} \cdot \text{m}^{-2} \cdot {}^\circ\text{C}^{-1}$)	Resistance ($\text{m}^2 \cdot {}^\circ\text{C} \cdot \text{W}^{-1}$)
River water	3000-12,000	0.0003-0.0001
Sea water	1000-3000	0.001-0.0003
Cooling water (towers)	3000-6000	0.0003-0.00017
Towns water (soft)	3000-5000	0.0003-0.0002
Towns water (hard)	1000-2000	0.001-0.0005
Steam condensate	1500-5000	0.00067-0.0002
Steam (oil free)	4000-10,000	0.0025-0.0001
Steam (oil traces)	2000-5000	0.0005-0.0002
Refrigerated brine	3000-5000	0.0003-0.0002
Air and industrial gases	5000-10,000	0.0002-0.0001
Flue gases	2000-5000	0.0005-0.0002
Organic vapors	5000	0.0002
Organic liquids	5000	0.0002
Light hydrocarbons	5000	0.0002
Heavy hydrocarbons	2000	0.0005
Boiling organics	2500	0.0004
Condensing organics	5000	0.0002
Heat transfer fluids	5000	0.0002
Aqueous salt solutions	3000-5000	0.0003-0.0002

10.9.2 Design Iteration

Since the calculated overall heat transfer coefficient ($U_{calculated} = 1450 \text{ W/m}^2 \cdot \text{K}$) differs significantly from our initial assumption ($U_{assumed} = 5000 \text{ W/m}^2 \cdot \text{K}$), we need to

iterate by assuming $U_{assumed} = U_{calculated}$ and recalculating the required area:

$$\begin{aligned} A &= \frac{Q}{U \times F \times LMTD} \\ &= \frac{15,205,555}{1450 \times 0.8760 \times 204.29} \\ &= \frac{15,205,555}{229,823} \\ &\approx 59 \text{ m}^2 \end{aligned}$$

This new area estimate would lead to a revised tube count, which would then affect the shell diameter and other parameters. This iterative process continues until convergence is achieved.

10.10 Final Heat Exchanger Design

After multiple iterations to converge on a consistent design, the final heat exchanger specifications are determined.

10.10.1 Final Heat Transfer Parameters

The converged heat transfer parameters are:

$$U = 1336 \text{ W/m}^2 \cdot \text{K} \quad (\text{overall heat transfer coefficient})$$

$$A = 64 \text{ m}^2 \quad (\text{total heat transfer area})$$

$$N_{tubes} = 135 \text{ tubes} \quad (\text{total number of tubes})$$

The final bundle and shell diameters are calculated based on the converged number of tubes:

$$\begin{aligned} D_b &= d_o \times \left(\frac{N_{tubes}}{0.249} \right)^{1/2.207} \\ &= 0.025 \times \left(\frac{135}{0.249} \right)^{1/2.207} \\ &\approx 0.43 \text{ m} \end{aligned}$$

The final shell diameter:

$$\begin{aligned} D_s &= D_b + 0.01 \\ &= 0.43 + 0.01 \\ &= 0.44 \text{ m} \end{aligned}$$

10.11 Conclusion

The final Parameter of the Shell and tube heat exchanger are given in the Tabel 10.6

Table 10.3: Final Heat Exchanger Design Parameters

Parameter	Value	Unit
Tube outer diameter	25	mm
Tube inner diameter	21	mm
Tube length	6.10	m
Number of tubes	135	-
Tube arrangement	Triangular pattern	-
Shell diameter	440	mm
Overall heat transfer coefficient	1336	W/m ² .K
Total heat transfer area	64	m ²
Number of Chamber	27	-
Actual Baffle Spacing (b)	0.22	m

Table 10.4: Process Stream Conditions

	Temperature (°C)	Compounds
Stream 1	50	Paraffin, Hydrogen
Stream 2	250	Paraffin, Hydrogen
Stream 4	425	Paraffin, Olefin, Hydrogen
Stream 5	286	Paraffin, Olefin, Hydrogen

Item	Thickness (in mm)
Benzene	15
Alkane	17
LAB	30
HAB	8

Item	Hold up time	Diameter (m)	Height (m)	Volume (m ³)
Benzene	24 Hrs	5.72	6	155
Alkane	24 Hrs	8.36	7.44	410
LAB	10 days	22.34	12.4	4860
HAB	10 days	5.75	6.1	160

Table 10.5: Process Stream Conditions

	Temperature (°C)	Compounds
Stream 1	50	Paraffin, Hydrogen
Stream 2	250	Paraffin, Hydrogen
Stream 4	425	Paraffin, Olefin, Hydrogen
Stream 5	286	Paraffin, Olefin, Hydrogen

- **Depreciation per year** = Rs 24.5 Crore
- **Taxation Rate** = 27.5%

Profit Calculations:

Gross Profit before Depreciation = Revenue – Total Product Cost

$$\text{Net Profit} = (\text{Gross Profit} - \text{Depreciation}) \times (1 - \text{Tax Rate})$$

$$N_{\min} = \frac{\ln \left(\frac{x_{D,LK} \cdot x_{B,HK}}{x_{B,LK} \cdot x_{D,HK}} \right)}{\ln \alpha_{LK,HK}} - 1 \quad (10.1)$$

Relative Volatility:

$$\alpha_{LK,HK}(T) = \frac{K_{LK}(T)}{K_{HK}(T)} \quad (10.2)$$

Feed Quality Line:

$$(1 - q) = \sum_i \frac{\alpha_{i,HK} \cdot x_{F,i}}{\alpha_{i,HK} - A} \quad (10.3)$$

Table 10.6: Final Heat Exchanger Design Parameters

Parameter	Value	Unit
Tube outer diameter	25	mm
Tube inner diameter	21	mm
Tube length	6.10	m
Number of tubes	135	-
Tube arrangement	Triangular pattern	-
Shell diameter	440	mm
LMTD	204	°C
Overall heat transfer coefficient	1336	W/m ² .K
Total heat transfer area	64	m ²
Number of Chamber	27	-
Actual Baffle Spacing (b)	0.22	m

Cost / Revenue Item	Amount (Rs Crore)
Total Equipment Cost	54
Total Capital Investment (Includes direct, indirect and working capital)	323
Raw Material	1003
Total Product Cost (Includes Labour, Utilities, other miscellaneous charges)	2590
Maximum Revenue (100% plant capacity)	2655

Minimum Reflux Ratio:

$$R_m + 1 = \frac{V}{D} = \sum_i \frac{\alpha_{i, HK} \cdot x_{D,i}}{\alpha_{i, HK} - A} \quad (10.4)$$

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